

Name	Synonym	Mol. Form.	CAS Reg. No.	Mol. Wt.	Step	<i>t</i> /°C	p <i>K</i> _s
Acetaldehyde	Ethanal	C ₂ H ₄ O	75-07-0	44.052		25	13.57
Acetamide	Ethanamide	C ₂ H ₅ NO	60-35-5	59.067		25	15.1
Acetanilide	<i>N</i> -Phenylacetamide	C ₈ H ₉ NO	103-84-4	135.163		25	0.5
Acetazolamide	<i>N</i> -[5-(Aminosulfonyl)-1,3,4-thiadiazol-2-yl]acetamide	C ₄ H ₆ N ₄ O ₅ S ₂	59-66-5	222.246			7.2
Acetic acid	Ethanoic acid	C ₂ H ₄ O ₂	64-19-7	60.052		25	4.756
Acetoacetic acid		C ₄ H ₆ O ₃	541-50-4	102.089		25	3.6
Acetohydroxamic acid	<i>N</i> -Hydroxyacetamide	C ₂ H ₅ NO ₂	546-88-3	75.067			8.70
<i>N</i> -Acetylglycine	Aceturic acid	C ₆ H ₇ NO ₃	543-24-8	117.104		25	3.67
2-(Acetyloxy)benzoic acid	Acetylsalicylic acid	C ₉ H ₈ O ₄	50-78-2	180.158		25	3.48
Aconine		C ₂₅ H ₄₁ NO ₉	509-20-6	499.596			9.52
Aconitine		C ₃₄ H ₄₇ NO ₁₁	302-27-2	645.737			5.88
9-Acerdinamine	Aminacrine	C ₁₃ H ₁₀ N ₂	90-45-9	194.231		20	9.99
Acridine	Dibenzo[<i>b,e</i>]pyridine	C ₁₃ H ₉ N	260-94-6	179.217		20	5.58
3,6-Acridinediamine	Proflavine	C ₁₃ H ₁₁ N ₃	92-62-6	209.246		20	9.65
Acrylic acid	2-Propenoic acid	C ₃ H ₄ O ₂	79-10-7	72.063		25	4.25
Adenine	1 <i>H</i> -Purin-6-amine	C ₅ H ₅ N ₅	73-24-5	135.128	1		4.3
Adenine	1 <i>H</i> -Purin-6-amine	C ₅ H ₅ N ₅	73-24-5	135.128	2		9.83
Adenosine	β - <i>D</i> -Ribofuranoside, adenine-9	C ₁₀ H ₁₃ N ₅ O ₄	58-61-7	267.242	1	25	3.6
Adenosine	β - <i>D</i> -Ribofuranoside, adenine-9	C ₁₀ H ₁₃ N ₅ O ₄	58-61-7	267.242	2	25	12.4
5'-Adenylic acid	Adenosine 5'-monophosphate	C ₁₀ H ₁₄ N ₅ O ₇ P	61-19-8	347.222	1		3.8
5'-Adenylic acid	Adenosine 5'-monophosphate	C ₁₀ H ₁₄ N ₅ O ₇ P	61-19-8	347.222	2		6.2
Adipamic acid		C ₈ H ₁₁ NO ₃	334-25-8	145.156		25	4.63
Agaritin	<i>L</i> -Glutamic acid, 5-[2-[4-(hydroxymethyl)phenyl]hydrazide]	C ₁₂ H ₁₇ N ₃ O ₄	2757-90-6	267.281	1		3.4
Agaritin	<i>L</i> -Glutamic acid, 5-[2-[4-(hydroxymethyl)phenyl]hydrazide]	C ₁₂ H ₁₇ N ₃ O ₄	2757-90-6	267.281	2		8.86
<i>L</i> -Alanine	2-Aminopropanoic acid, (<i>S</i> -)	C ₃ H ₇ NO ₂	56-41-7	89.094	1	25	2.34
<i>L</i> -Alanine	2-Aminopropanoic acid, (<i>S</i> -)	C ₃ H ₇ NO ₂	56-41-7	89.094	2	25	9.87
β -Alanine	3-Aminopropanoic acid	C ₃ H ₇ NO ₂	107-95-9	89.094	1	25	3.55
β -Alanine	3-Aminopropanoic acid	C ₃ H ₇ NO ₂	107-95-9	89.094	2	25	10.24
Allantoin		C ₄ H ₆ N ₄ O ₃	97-59-6	158.116		25	8.96
Allopurinol	1,5-Dihydro-4 <i>H</i> -pyrazolo[3,4- <i>d</i>]pyrimidin-4-one	C ₅ H ₄ N ₄ O	315-30-0	136.112			10.2
Alloxanic acid		C ₄ H ₄ N ₂ O ₅	470-44-0	160.085		25	6.64
Allyl alcohol	2-Propen-1-ol	C ₃ H ₆ O	107-18-6	58.079		25	15.5
Allylamine	2-Propen-1-amine	C ₃ H ₇ N	107-11-9	57.095		25	9.49
<i>N</i> -Allylaniline	Allylphenylamine	C ₈ H ₁₁ N	589-09-3	133.190		25	4.17
Aminoacetonitrile		C ₂ H ₄ N ₂	540-61-4	56.066		25	5.34
2-Amino adipic acid		C ₆ H ₁₁ NO ₄	626-71-1	161.156	1	25	2.14
2-Amino adipic acid		C ₆ H ₁₁ NO ₄	626-71-1	161.156	2	25	4.21
2-Amino adipic acid		C ₆ H ₁₁ NO ₄	626-71-1	161.156	3	25	9.77
4-Aminoazobenzene		C ₁₂ H ₁₁ N ₃	60-09-3	197.235		25	2.82
2-Aminobenzenesulfonic acid	Orthanilic acid	C ₆ H ₇ NO ₃ S	88-21-1	173.190		25	2.46
3-Aminobenzenesulfonic acid	Metanilic acid	C ₆ H ₇ NO ₃ S	121-47-1	173.190		25	3.74
4-Aminobenzenesulfonic acid	Sulfanilic acid	C ₆ H ₇ NO ₃ S	121-57-3	173.190		25	3.23
2-Aminobenzonitrile		C ₇ H ₆ N ₂	1885-29-6	118.136		25	0.77
3-Aminobenzonitrile		C ₇ H ₆ N ₂	2237-30-1	118.136		25	2.75
4-Aminobenzonitrile		C ₇ H ₆ N ₂	873-74-5	118.136		25	1.74
2-Aminobiphenyl		C ₁₂ H ₁₁ N	90-41-5	169.222		25	3.83
3-Aminobiphenyl		C ₁₂ H ₁₁ N	2243-47-2	169.222		18	4.25
4-Aminobiphenyl	<i>p</i> -Biphenylamine	C ₁₂ H ₁₁ N	92-67-1	169.222		18	4.35
<i>DL</i> -2-Aminobutanoic acid		C ₄ H ₉ NO ₂	2835-81-6	103.120	1	25	2.29
<i>DL</i> -2-Aminobutanoic acid		C ₄ H ₉ NO ₂	2835-81-6	103.120	2	25	9.83
4-Aminobutanoic acid	γ -Aminobutyric acid	C ₄ H ₉ NO ₂	56-12-2	103.120	1	25	4.031
4-Aminobutanoic acid	γ -Aminobutyric acid	C ₄ H ₉ NO ₂	56-12-2	103.120	2	25	10.556
2-Aminoethanesulfonic acid	Taurine	C ₂ H ₇ NO ₃ S	107-35-7	125.147	1	25	1.5
2-Aminoethanesulfonic acid	Taurine	C ₂ H ₇ NO ₃ S	107-35-7	125.147	2	25	9.06
4-(2-Aminoethyl)phenol	Tyramine	C ₈ H ₁₁ NO	51-67-2	137.179	1	25	9.74
4-(2-Aminoethyl)phenol	Tyramine	C ₈ H ₁₁ NO	51-67-2	137.179	2	25	10.52
6-Aminohexanoic acid	ϵ -Aminocaproic acid	C ₆ H ₁₃ NO ₂	60-32-2	131.173	1	25	4.37
6-Aminohexanoic acid	ϵ -Aminocaproic acid	C ₆ H ₁₃ NO ₂	60-32-2	131.173	2	25	10.80

4-Amino-2-hydroxybenzoic acid	<i>p</i> -Aminosalicylic acid	C ₇ H ₇ NO ₃	65-49-6	153.136			3.25
2-Amino-4-hydroxypteridine		C ₆ H ₅ N ₅ O	2236-60-4	163.137	1	20	2.27
2-Amino-4-hydroxypteridine		C ₆ H ₅ N ₅ O	2236-60-4	163.137	2	20	7.96
5-Amino-1-naphthol	1-Amino-6-hydroxynaphthalene	C ₁₀ H ₉ NO	83-55-6	159.184		25	3.97
5-Amino-4-oxopentanoic acid	5-Aminolevulinic acid	C ₅ H ₉ NO ₃	106-60-5	131.130	1	25	4.05
5-Amino-4-oxopentanoic acid	5-Aminolevulinic acid	C ₅ H ₉ NO ₃	106-60-5	131.130	2	25	8.90
5-Aminopentanoic acid		C ₅ H ₁₁ NO ₂	660-88-8	117.147	1	25	4.27
5-Aminopentanoic acid		C ₅ H ₁₁ NO ₂	660-88-8	117.147	2	25	10.77
2-Aminophenol		C ₆ H ₇ NO	95-55-6	109.126	1	20	4.78
2-Aminophenol		C ₆ H ₇ NO	95-55-6	109.126	2	20	9.97
3-Aminophenol		C ₆ H ₇ NO	591-27-5	109.126	1	20	4.37
3-Aminophenol		C ₆ H ₇ NO	591-27-5	109.126	2	20	9.82
4-Aminophenol		C ₆ H ₇ NO	123-30-8	109.126	1	25	5.48
4-Aminophenol		C ₆ H ₇ NO	123-30-8	109.126	2	25	10.30
3-Aminopropanenitrile	3-Aminopropionitrile	C ₃ H ₆ N ₂	151-18-8	70.093		20	7.80
4-Amino-3,5,6-trichloro-2-pyridinecarboxylic acid	Picloram	C ₆ H ₃ Cl ₃ N ₂ O ₂	1918-02-1	241.459			3.6
Amiodarone		C ₂₃ H ₂₉ I ₂ NO ₃	1951-25-3	645.312		25	6.56
Amitriptyline		C ₂₀ H ₂₃ N	50-48-6	277.404			9.4
Amobarbital	5-Ethyl-5-isopentyl-2,4,6-(1 <i>H</i> ,3 <i>H</i> ,5 <i>H</i>)-pyrimidinetrione	C ₁₁ H ₁₈ N ₂ O ₃	57-43-2	226.272		25	8.0
Aniline	Benzenamine	C ₆ H ₇ N	62-53-3	93.127		25	4.87
Aniline-2-carboxylic acid	<i>o</i> -Anthranilic acid	C ₇ H ₇ NO ₂	118-92-3	137.137	1	25	2.17
Aniline-2-carboxylic acid	<i>o</i> -Anthranilic acid	C ₇ H ₇ NO ₂	118-92-3	137.137	2	25	4.85
Aniline-3-carboxylic acid	<i>m</i> -Anthranilic acid	C ₇ H ₇ NO ₂	99-05-8	137.137	1	25	3.07
Aniline-3-carboxylic acid	<i>m</i> -Anthranilic acid	C ₇ H ₇ NO ₂	99-05-8	137.137	2	25	4.79
Aniline-4-carboxylic acid	<i>p</i> -Anthranilic acid	C ₇ H ₇ NO ₂	150-13-0	137.137	1	25	2.50
Aniline-4-carboxylic acid	<i>p</i> -Anthranilic acid	C ₇ H ₇ NO ₂	150-13-0	137.137	2	25	4.87
Apomorphine		C ₁₇ H ₁₇ NO ₂	58-00-4	267.323	1		7.0
Apomorphine		C ₁₇ H ₁₇ NO ₂	58-00-4	267.323	2		8.92
Arcoline		C ₈ H ₁₃ NO ₂	63-75-2	155.195			6.84
<i>L</i> -Arginine		C ₆ H ₁₄ N ₄ O ₂	74-79-3	174.201	1	25	1.82
<i>L</i> -Arginine		C ₆ H ₁₄ N ₄ O ₂	74-79-3	174.201	2	25	8.99
<i>L</i> -Arginine		C ₆ H ₁₄ N ₄ O ₂	74-79-3	174.201	3	25	12.5
<i>L</i> -Argininosuccinic acid		C ₁₀ H ₁₈ N ₄ O ₅	2387-71-5	274.274	1	25	1.62
<i>L</i> -Argininosuccinic acid		C ₁₀ H ₁₈ N ₄ O ₅	2387-71-5	274.274	2	25	2.70
<i>L</i> -Argininosuccinic acid		C ₁₀ H ₁₈ N ₄ O ₅	2387-71-5	274.274	3	25	4.26
<i>L</i> -Argininosuccinic acid		C ₁₀ H ₁₈ N ₄ O ₅	2387-71-5	274.274	4	25	9.58
<i>L</i> -Ascorbic acid	Vitamin C	C ₆ H ₈ O ₆	50-81-7	176.124	1	25	4.04
<i>L</i> -Ascorbic acid	Vitamin C	C ₆ H ₈ O ₆	50-81-7	176.124	2	16	11.7
<i>L</i> -Asparagine	α -Aminosuccinamic acid	C ₄ H ₈ N ₂ O ₃	70-47-3	132.118	1	20	2.1
<i>L</i> -Asparagine	α -Aminosuccinamic acid	C ₄ H ₈ N ₂ O ₃	70-47-3	132.118	2	20	8.80
<i>L</i> -Aspartic acid	<i>L</i> -Aminosuccinic acid	C ₄ H ₇ NO ₄	56-84-8	133.104	1	25	1.99
<i>L</i> -Aspartic acid	<i>L</i> -Aminosuccinic acid	C ₄ H ₇ NO ₄	56-84-8	133.104	2	25	3.90
<i>L</i> -Aspartic acid	<i>L</i> -Aminosuccinic acid	C ₄ H ₇ NO ₄	56-84-8	133.104	3	25	9.90
Aspergilliacid		C ₁₂ H ₂₀ N ₂ O ₂	490-02-8	224.299			5.5
Atenolol		C ₁₄ H ₂₂ N ₂ O ₃	29122-68-7	266.336			9.6
Atisine	Anthorine	C ₂₂ H ₃₃ NO ₂	466-43-3	343.503			12.2
Azaserine		C ₅ H ₇ N ₃ O ₄	115-02-6	173.128			8.55
Azathioprine	1 <i>H</i> -Purine, 6-[(1-methyl-4-nitro-1 <i>H</i> -imidazol-5-yl)thio]-	C ₉ H ₇ N ₇ O ₂ S	446-86-6	277.263			8.2
6-Azauridine	2- β - <i>D</i> -Ribofuranosyl-1,2,4-triazine-3,5-(2 <i>H</i> ,4 <i>H</i>)-dione	C ₈ H ₁₁ N ₃ O ₆	54-25-1	245.189			6.70
Azetidine		C ₃ H ₇ N	503-29-7	57.095		25	11.29
Barbital	5,5-Diethylbarbituric acid	C ₈ H ₁₂ N ₂ O ₃	57-44-3	184.192		25	7.43
Barbituric acid		C ₄ H ₄ N ₂ O ₃	67-52-7	128.086		25	4.01
Benzaldehyde	Benzenecarboxaldehyde	C ₇ H ₆ O	100-52-7	106.122		25	14.90
Benzamide	Benzoic acid amide	C ₇ H ₇ NO	55-21-0	121.137		25	\approx 13
Benzenoacetic acid	Phenylacetic acid	C ₈ H ₈ O ₂	103-82-2	136.149		25	4.31
Benzeneboronic acid		C ₆ H ₇ BO ₂	98-80-6	121.930			8.83
Benzenebutanoic acid		C ₁₀ H ₁₂ O ₂	1821-12-1	164.201		25	4.76
1,2-Benzenediamine	<i>o</i> -Phenylenediamine	C ₆ H ₈ N ₂	95-54-5	108.141	1	20	4.57
1,2-Benzenediamine	<i>o</i> -Phenylenediamine	C ₆ H ₈ N ₂	95-54-5	108.141	2	20	0.80

1,3-Benzenediamine	<i>m</i> -Phenylenediamine	C ₆ H ₈ N ₂	108-45-2	108.141	1	20	5.11
1,3-Benzenediamine	<i>m</i> -Phenylenediamine	C ₆ H ₈ N ₂	108-45-2	108.141	2	20	2.50
1,4-Benzenediamine	<i>p</i> -Phenylenediamine	C ₆ H ₈ N ₂	106-50-3	108.141	1	20	6.31
1,4-Benzenediamine	<i>p</i> -Phenylenediamine	C ₆ H ₈ N ₂	106-50-3	108.141	2	20	2.97
Benzeneethanamine	2-Phenylethylamine	C ₈ H ₁₁ N	64-04-0	121.180		25	9.83
Benzenemethanethiol	Thiobenzyl alcohol	C ₇ H ₈ S	100-53-8	124.204		25	9.43
Benzenepropanoic acid	Hydrocinnamic acid	C ₉ H ₁₀ O ₂	501-52-0	150.174		25	4.66
Benzenesulfonic acid		C ₆ H ₆ O ₂ S	618-41-7	142.176		20	1.3
Benzenesulfonic acid	Besyllic acid	C ₆ H ₆ O ₃ S	98-11-3	158.175		25	0.70
Benzenethiol	Phenyl mercaptan	C ₆ H ₆ S	108-98-5	110.177		25	6.62
<i>p</i> -Benzidine	[1,1'-Biphenyl]-4,4'-diamine	C ₁₂ H ₁₂ N ₂	92-87-5	184.236	1	20	4.65
<i>p</i> -Benzidine	[1,1'-Biphenyl]-4,4'-diamine	C ₁₂ H ₁₂ N ₂	92-87-5	184.236	2	20	3.43
1 <i>H</i> -Benzimidazole	<i>N,N'</i> -Methenyl- <i>o</i> -phenylenediamine	C ₇ H ₈ N ₂	51-17-2	118.136		25	5.53
Benzoic acid	Benzenecarboxylic acid	C ₇ H ₆ O ₂	65-85-0	122.122		25	4.204
1 <i>H</i> -Benzotriazole	1,2,3-Triaza-1 <i>H</i> -indene	C ₆ H ₅ N ₃	95-14-7	119.124		20	1.6
<i>N</i> -Benzoylethylglycine	Hippuric acid	C ₈ H ₉ NO ₃	495-69-2	179.172		25	3.62
Benzpiperlylon	1,2-Dihydro-2-(1-methyl-4-piperidinyl)-5-phenyl-4-benzyl-3 <i>H</i> -pyrazol-3-one	C ₂₂ H ₂₅ N ₃ O	53-89-4	347.453	1		6.73
Benzpiperlylon	1,2-Dihydro-2-(1-methyl-4-piperidinyl)-5-phenyl-4-benzyl-3 <i>H</i> -pyrazol-3-one	C ₂₂ H ₂₅ N ₃ O	53-89-4	347.453	2		9.13
Benzylamine	Benzenemethanamine	C ₇ H ₉ N	100-46-9	107.153		25	9.34
4-Benzylaniline		C ₁₃ H ₁₃ N	1135-12-2	183.249		25	2.17
2-Benzylpyridine		C ₁₂ H ₁₁ N	101-82-6	169.222		25	5.13
Betaine	1-Carboxy- <i>N,N,N</i> -trimethylmethanaminium, inner salt	C ₅ H ₁₁ NO ₂	107-43-7	117.147		0	1.83
Biguanide	Imidodicarbonimidic diamide	C ₂ H ₇ N ₅	56-03-1	101.111	1		11.52
Biguanide	Imidodicarbonimidic diamide	C ₂ H ₇ N ₅	56-03-1	101.111	2		2.93
<i>N,N</i> -Bis(2-hydroxyethyl)glycine	Bicine	C ₆ H ₁₃ NO ₄	150-25-4	163.172	2	20	8.35
Bithionol		C ₁₂ H ₆ Cl ₄ O ₂ S	97-18-7	356.052	1		4.82
Bithionol		C ₁₂ H ₆ Cl ₄ O ₂ S	97-18-7	356.052	2		10.50
Bornylamine	1,7,7-Trimethylbicyclo[2.2.1]heptan-2-amine, (1 <i>R</i> -endo)-	C ₁₀ H ₁₉ N	32511-34-5	153.265		25	10.17
Bromadiolone		C ₃₀ H ₂₃ BrO ₄	28772-56-7	527.406		21	4.04
Bromoacetic acid		C ₂ H ₃ BrO ₂	79-08-3	138.948		25	2.90
2-Bromoaniline		C ₆ H ₆ BrN	615-36-1	172.023		25	2.53
3-Bromoaniline		C ₆ H ₆ BrN	591-19-5	172.023		25	3.53
4-Bromoaniline		C ₆ H ₆ BrN	106-40-1	172.023		25	3.89
2-Bromobenzoic acid		C ₇ H ₅ BrO ₂	88-65-3	201.018		25	2.85
3-Bromobenzoic acid		C ₇ H ₅ BrO ₂	585-76-2	201.018		25	3.81
4-Bromobenzoic acid		C ₇ H ₅ BrO ₂	586-76-5	201.018		25	3.96
Bromocresol Green	Bromocresol Green	C ₂₁ H ₁₄ Br ₄ O ₅ S	76-60-8	698.014			4.7
Bromocresol Purple	Bromocresol Purple	C ₂₁ H ₁₆ Br ₂ O ₅ S	115-40-2	540.222			6.3
4-Bromo- <i>N,N</i> -dimethylaniline		C ₈ H ₁₀ BrN	586-77-6	200.076		25	4.23
2-Bromophenol		C ₆ H ₅ BrO	95-56-7	173.007		25	8.45
3-Bromophenol		C ₆ H ₅ BrO	591-20-8	173.007		25	9.03
4-Bromophenol		C ₆ H ₅ BrO	106-41-2	173.007		25	9.37
Bromophenol Blue	Bromphenol Blue	C ₁₉ H ₁₀ Br ₄ O ₅ S	115-39-9	669.960			4.0
3-Bromopropanoic acid	β -Bromopropionic acid	C ₃ H ₅ BrO ₂	590-92-1	152.975		25	4.00
3-Bromopyridine		C ₅ H ₄ BrN	626-55-1	157.997		25	2.84
3-Bromoquinoline		C ₉ H ₆ BrN	5332-24-1	208.055		25	2.69
Bromothymol Blue	Bromthymol Blue	C ₂₇ H ₂₈ Br ₂ O ₅ S	76-59-5	624.381			7.0
Brucine		C ₂₃ H ₂₆ N ₂ O ₄	357-57-3	394.463	1		6.04
Brucine		C ₂₃ H ₂₆ N ₂ O ₄	357-57-3	394.463	2		11.07
1,4-Butanediamine	Putrescine	C ₄ H ₁₂ N ₂	110-60-1	88.151	1	25	10.80
1,4-Butanediamine	Putrescine	C ₄ H ₁₂ N ₂	110-60-1	88.151	2	25	9.63
1,2,3,4-Butanetetrol	Erythritol	C ₄ H ₁₀ O ₄	149-32-6	122.120			13.9
Butanoic acid	Butyric acid	C ₄ H ₈ O ₂	107-92-6	88.106		25	4.83
<i>trans</i> -2-Butenoic acid	Crotonic acid	C ₄ H ₆ O ₂	107-93-7	86.090		25	4.69
3-Butenoic acid		C ₄ H ₆ O ₂	625-38-7	86.090		25	4.34

Butylamine	1-Butanamine	C ₄ H ₁₁ N	109-73-9	73.137		25	10.60
sec-Butylamine	2-Butanamine, (±)-	C ₄ H ₁₁ N	33966-50-6	73.137		25	10.56
tert-Butylamine	2-Methyl-2-propanamine	C ₄ H ₁₁ N	75-64-9	73.137		25	10.68
N-tert-Butylaniline		C ₁₀ H ₁₅ N	937-33-7	149.233		25	7.00
2-tert-Butylbenzoic acid		C ₁₁ H ₁₄ O ₂	1077-58-3	178.228		25	3.54
3-tert-Butylbenzoic acid		C ₁₁ H ₁₄ O ₂	7498-54-6	178.228		25	4.20
4-tert-Butylbenzoic acid		C ₁₁ H ₁₄ O ₂	98-73-7	178.228		25	4.38
Butylcyclohexylamine	N-Butylcyclohexanamine	C ₁₀ H ₂₁ N	10108-56-2	155.281		25	11.23
2-tert-Butylphenol		C ₁₀ H ₁₄ O	88-18-6	150.217		25	10.62
3-tert-Butylphenol		C ₁₀ H ₁₄ O	585-34-2	150.217		25	10.12
4-tert-Butylphenol		C ₁₀ H ₁₄ O	98-54-4	150.217		25	10.23
N-Butylpiperidine		C ₉ H ₁₉ N	4945-48-6	141.254		23	10.47
Butylpropanedioic acid	Butylmalonic acid	C ₇ H ₁₂ O ₄	534-59-8	160.168	1	5	2.96
2-Butynoic acid		C ₄ H ₆ O ₂	590-93-2	84.074		25	2.62
Captopril	1-(3-Mercapto-2-methyl-1-oxopropyl)proline	C ₉ H ₁₅ NO ₃ S	62571-86-2	217.285	1		3.7
Captopril	1-(3-Mercapto-2-methyl-1-oxopropyl)proline	C ₉ H ₁₅ NO ₃ S	62571-86-2	217.285	2		9.8
Carbamodithioic acid		CH ₃ NS ₂	594-07-0	93.172		25	2.95
Carbendazim	Carbamic acid, 1 <i>H</i> -benzimidazol-2-yl-, methyl ester	C ₉ H ₉ N ₃ O ₂	10605-21-7	191.186			4.48
L-γ-Carboxyglutamic acid		C ₆ H ₉ NO ₆	53861-57-7	191.138	1	25	1.7
L-γ-Carboxyglutamic acid		C ₆ H ₉ NO ₆	53861-57-7	191.138	2	25	3.2
L-γ-Carboxyglutamic acid		C ₆ H ₉ NO ₆	53861-57-7	191.138	3	25	4.75
L-γ-Carboxyglutamic acid		C ₆ H ₉ NO ₆	53861-57-7	191.138	4	25	9.9
Carnitine	4-Amino-3-hydroxybutanoic acid trimethylbetaine	C ₇ H ₁₅ NO ₃	541-15-1	161.199		25	3.80
Carnosine	N-β-Alanyl-L-histidine	C ₉ H ₁₄ N ₄ O ₃	305-84-0	226.232	1	20	2.73
Carnosine	N-β-Alanyl-L-histidine	C ₉ H ₁₄ N ₄ O ₃	305-84-0	226.232	2	20	6.87
Carnosine	N-β-Alanyl-L-histidine	C ₉ H ₁₄ N ₄ O ₃	305-84-0	226.232	3	20	9.73
Cephalexin		C ₁₆ H ₁₇ N ₃ O ₄ S	15686-71-2	347.389	1		5.2
Cephalexin		C ₁₆ H ₁₇ N ₃ O ₄ S	15686-71-2	347.389	2		7.3
Cephaloridine		C ₁₉ H ₁₇ N ₃ O ₄ S ₂	50-59-9	415.486			3.2
Cephradine		C ₁₆ H ₁₉ N ₃ O ₄ S	38821-53-3	349.405	1		2.63
Cephradine		C ₁₆ H ₁₉ N ₃ O ₄ S	38821-53-3	349.405	2		7.27
Chloroacetic acid		C ₂ H ₃ ClO ₂	79-11-8	94.497		25	2.87
2-Chloroaniline		C ₆ H ₆ ClN	95-51-2	127.572		25	2.66
3-Chloroaniline		C ₆ H ₆ ClN	108-42-9	127.572		25	3.52
4-Chloroaniline		C ₆ H ₆ ClN	106-47-8	127.572		25	3.98
2-Chlorobenzoic acid		C ₈ H ₇ ClO ₂	2444-36-2	170.594		25	4.07
3-Chlorobenzoic acid		C ₈ H ₇ ClO ₂	1878-65-5	170.594		25	4.14
4-Chlorobenzoic acid		C ₈ H ₇ ClO ₂	1878-66-6	170.594		25	4.19
2-Chlorobenzoic acid		C ₇ H ₅ ClO ₂	118-91-2	156.567		25	2.90
3-Chlorobenzoic acid		C ₇ H ₅ ClO ₂	535-80-8	156.567		25	3.84
4-Chlorobenzoic acid		C ₇ H ₅ ClO ₂	74-11-3	156.567		25	4.00
2-Chlorobutanoic acid		C ₆ H ₇ ClO ₂	4170-24-5	122.551			2.86
3-Chlorobutanoic acid		C ₆ H ₇ ClO ₂	625-68-3	122.551			4.05
4-Chlorobutanoic acid		C ₆ H ₇ ClO ₂	627-00-9	122.551			4.52
trans-o-Chlorocinnamic acid		C ₉ H ₇ ClO ₂	939-58-2	182.604		25	4.23
trans-m-Chlorocinnamic acid		C ₉ H ₇ ClO ₂	14473-90-6	182.604		25	4.29
trans-p-Chlorocinnamic acid		C ₉ H ₇ ClO ₂	940-62-5	182.604		25	4.41
Chlorodiazepoxide	7-Chloro-N-methyl-5-phenyl-3 <i>H</i> -1,4-benzodiazepin-2-amine, 4-oxide	C ₁₆ H ₁₄ ClN ₃ O	58-25-3	299.754			4.8
3-Chloro-N,N-dimethylaniline		C ₈ H ₁₀ ClN	6848-13-1	155.625		20	3.83
4-Chloro-N,N-dimethylaniline		C ₈ H ₁₀ ClN	698-69-1	155.625		20	4.39
2-Chlorophenol		C ₆ H ₅ ClO	95-57-8	128.556		25	8.56
3-Chlorophenol		C ₆ H ₅ ClO	108-43-0	128.556		25	9.12
4-Chlorophenol		C ₆ H ₅ ClO	106-48-9	128.556		25	9.41
2-Chlorophenoxyacetic acid		C ₈ H ₇ ClO ₃	614-61-9	186.593		25	3.05
3-Chlorophenoxyacetic acid		C ₈ H ₇ ClO ₃	588-32-9	186.593		25	3.10
3-(2-Chlorophenyl)propanoic acid		C ₉ H ₉ ClO ₂	1643-28-3	184.619		25	4.58
3-(3-Chlorophenyl)propanoic acid		C ₉ H ₉ ClO ₂	21640-48-2	184.619		25	4.59

3-(4-Chlorophenyl)propanoic acid		C ₉ H ₉ ClO ₂	2019-34-3	184.619		25	4.61
2-Chloropropanoic acid	2-Chloropropionic acid	C ₃ H ₅ ClO ₂	598-78-7	108.524		25	2.83
3-Chloropropanoic acid	β-Chloropropionic acid	C ₃ H ₅ ClO ₂	107-94-8	108.524		25	3.98
2-Chloropyridine		C ₅ H ₄ ClN	109-09-1	113.546		25	0.49
3-Chloropyridine		C ₅ H ₄ ClN	626-60-8	113.546		25	2.81
4-Chloropyridine		C ₅ H ₄ ClN	626-61-9	113.546		25	3.83
Chlorothiazide		C ₇ H ₆ ClN ₃ O ₄ S ₂	58-94-6	295.724	1		6.85
Chlorothiazide		C ₇ H ₆ ClN ₃ O ₄ S ₂	58-94-6	295.724	2		9.45
Cholic acid	3,7,12-Trihydroxycolan-24-oic acid, (3α,5β,7α,12α)	C ₂₄ H ₄₀ O ₅	81-25-4	408.572			6.4
Choline		C ₅ H ₁₄ NO	62-49-7	104.171		25	13.9
Cinchonidine		C ₁₉ H ₂₂ N ₂ O	485-71-2	294.390	1		5.80
Cinchonidine		C ₁₉ H ₂₂ N ₂ O	485-71-2	294.390	2		10.03
Cinchonine		C ₁₉ H ₂₂ N ₂ O	118-10-5	294.390	1		5.85
Cinchonine		C ₁₉ H ₂₂ N ₂ O	118-10-5	294.390	2		9.92
<i>cis</i> -Cinnamic acid	3-Phenyl-2-propenoic acid, (Z)-	C ₉ H ₈ O ₂	102-94-3	148.159		25	3.88
<i>trans</i> -Cinnamic acid	3-Phenyl-2-propenoic acid, (E)-	C ₉ H ₈ O ₂	140-10-3	148.159		25	4.44
Cinnoline	1,2-Benzodiazine	C ₈ H ₆ N ₂	253-66-7	130.147		20	2.37
Citric acid	2-Hydroxy-1,2,3-propanetricarboxylic acid	C ₆ H ₈ O ₇	77-92-9	192.124	1	25	3.13
Citric acid	2-Hydroxy-1,2,3-propanetricarboxylic acid	C ₆ H ₈ O ₇	77-92-9	192.124	2	25	4.76
Citric acid	2-Hydroxy-1,2,3-propanetricarboxylic acid	C ₆ H ₈ O ₇	77-92-9	192.124	3	25	6.40
Citrulline	<i>N</i> 5-(Aminocarbonyl)- <i>L</i> -ornithine	C ₆ H ₁₃ N ₃ O ₃	372-75-8	175.185	1	25	2.43
Citrulline	<i>N</i> 5-(Aminocarbonyl)- <i>L</i> -ornithine	C ₆ H ₁₃ N ₃ O ₃	372-75-8	175.185	2	25	9.69
Clindamycin		C ₁₈ H ₃₃ ClN ₇ O ₅ S	18323-44-9	424.983			7.6
Clonazepam		C ₁₅ H ₁₀ ClN ₃ O ₃	1622-61-3	315.711	1		1.5
Clonazepam		C ₁₅ H ₁₀ ClN ₃ O ₃	1622-61-3	315.711	2		10.5
Clozapine	Clozaril	C ₁₈ H ₁₉ ClN ₄	5786-21-0	326.824	1		3.70
Clozapine	Clozaril	C ₁₈ H ₁₉ ClN ₄	5786-21-0	326.824	2		7.60
Codeine		C ₁₈ H ₂₁ NO ₃	76-57-3	299.365			8.21
Colchicine		C ₂₂ H ₂₅ NO ₆	64-86-8	399.437		20	12.36
Creatine		C ₄ H ₉ N ₃ O ₂	57-00-1	131.133	1	25	2.63
Creatine		C ₄ H ₉ N ₃ O ₂	57-00-1	131.133	2	25	14.3
Creatinine		C ₄ H ₇ N ₃ O	60-27-5	113.118	1	25	4.8
Creatinine		C ₄ H ₇ N ₃ O	60-27-5	113.118	2		9.2
<i>o</i> -Cresol	2-Methylphenol	C ₇ H ₈ O	95-48-7	108.138		25	10.29
<i>m</i> -Cresol	3-Methylphenol	C ₇ H ₈ O	108-39-4	108.138		25	10.09
<i>p</i> -Cresol	4-Methylphenol	C ₇ H ₈ O	106-44-5	108.138		25	10.26
<i>o</i> -Cresolphthalein		C ₂₂ H ₁₈ O ₄	596-27-0	346.376			9.4
Cresol Red	<i>o</i> -Cresolsulphonphthalein	C ₂₁ H ₁₈ O ₅ S	1733-12-6	382.430			8.3
Cupreine		C ₁₉ H ₂₂ N ₂ O ₂	524-63-0	310.390			6.57
Cyanamide	Cyanogenamide	CH ₂ N ₂	420-04-2	42.040		29	1.1
Cyanic acid	Hydrogen cyanate	CHNO	420-05-3	43.025		25	3.7
Cyanoacetic acid		C ₃ H ₃ NO ₂	372-09-8	85.062		25	2.47
3-Cyanobenzoic acid		C ₈ H ₅ NO ₂	1877-72-1	147.132		25	3.60
4-Cyanobenzoic acid		C ₈ H ₅ NO ₂	619-65-8	147.132		25	3.55
4-Cyanobutanoic acid		C ₈ H ₇ NO ₂	39201-33-7	113.116		25	2.42
(2-Cyanophenoxy)acetic acid		C ₉ H ₇ NO ₃	6574-95-4	177.157		25	2.98
(3-Cyanophenoxy)acetic acid		C ₉ H ₇ NO ₃	1879-58-9	177.157		25	3.03
(4-Cyanophenoxy)acetic acid		C ₉ H ₇ NO ₃	1878-82-6	177.157		25	2.93
Cyanuric acid	1,3,5-Triazine-2,4,6(1 <i>H</i> ,3 <i>H</i> ,5 <i>H</i>)-trione	C ₃ H ₃ N ₃ O ₃	108-80-5	129.074	1		6.88
Cyanuric acid	1,3,5-Triazine-2,4,6(1 <i>H</i> ,3 <i>H</i> ,5 <i>H</i>)-trione	C ₃ H ₃ N ₃ O ₃	108-80-5	129.074	2		11.40
Cyanuric acid	1,3,5-Triazine-2,4,6(1 <i>H</i> ,3 <i>H</i> ,5 <i>H</i>)-trione	C ₃ H ₃ N ₃ O ₃	108-80-5	129.074	3		13.5
Cyclohexanecarboxylic acid	Hexahydrobenzoic acid	C ₇ H ₁₂ O ₂	98-89-5	128.169		25	4.91
<i>cis</i> -1,2-Cyclohexanediamine	<i>cis</i> -1,2-Diaminocyclohexane	C ₆ H ₁₄ N ₂	1436-59-5	114.188	1	20	9.93
<i>cis</i> -1,2-Cyclohexanediamine	<i>cis</i> -1,2-Diaminocyclohexane	C ₆ H ₁₄ N ₂	1436-59-5	114.188	2	20	6.13
<i>trans</i> -1,2-Cyclohexanediamine	<i>trans</i> -1,2-Diaminocyclohexane	C ₆ H ₁₄ N ₂	1121-22-8	114.188	1	20	9.94
<i>trans</i> -1,2-Cyclohexanediamine	<i>trans</i> -1,2-Diaminocyclohexane	C ₆ H ₁₄ N ₂	1121-22-8	114.188	2	20	6.47

1,3-Cyclohexanedione	Dihydroresorcinol	C ₆ H ₈ O ₂	504-02-9	112.127		25	5.26
Cyclohexylamine	Cyclohexanamine	C ₆ H ₁₃ N	108-91-8	99.174		25	10.64
Cyclopentanecarboxylic acid	Cyclopentanoic acid	C ₆ H ₁₀ O ₂	3400-45-1	114.142		25	4.99
Cyclopropanecarboxylic acid		C ₄ H ₆ O ₂	1759-53-1	86.090		25	4.83
1,1-Cyclopropanedicarboxylic acid		C ₃ H ₆ O ₄	598-10-7	130.100	1	25	1.82
1,1-Cyclopropanedicarboxylic acid		C ₃ H ₆ O ₄	598-10-7	130.100	2	25	7.43
Cysteamine		C ₂ H ₇ NS	60-23-1	77.149	1	25	8.27
Cysteamine		C ₂ H ₇ NS	60-23-1	77.149	2	25	10.53
DL-Cysteic acid		C ₃ H ₇ NO ₃ S	3024-83-7	169.157	1	25	1.3
DL-Cysteic acid		C ₃ H ₇ NO ₃ S	3024-83-7	169.157	2	25	1.9
DL-Cysteic acid		C ₃ H ₇ NO ₃ S	3024-83-7	169.157	3	25	8.70
L-Cysteine	Propanoic acid, 2-amino-3-mercapto-, (R)-	C ₃ H ₇ NO ₂ S	52-90-4	121.159	1	25	1.5
L-Cysteine	Propanoic acid, 2-amino-3-mercapto-, (R)-	C ₃ H ₇ NO ₂ S	52-90-4	121.159	2	25	8.7
L-Cysteine	Propanoic acid, 2-amino-3-mercapto-, (R)-	C ₃ H ₇ NO ₂ S	52-90-4	121.159	3	25	10.2
L-Cystine	3,3'-Dithiobis(2-aminopropanoic acid)	C ₆ H ₁₂ N ₂ O ₄ S ₂	56-89-3	240.300	1		1
L-Cystine	3,3'-Dithiobis(2-aminopropanoic acid)	C ₆ H ₁₂ N ₂ O ₄ S ₂	56-89-3	240.300	2		2.1
L-Cystine	3,3'-Dithiobis(2-aminopropanoic acid)	C ₆ H ₁₂ N ₂ O ₄ S ₂	56-89-3	240.300	3		8.02
L-Cystine	3,3'-Dithiobis(2-aminopropanoic acid)	C ₆ H ₁₂ N ₂ O ₄ S ₂	56-89-3	240.300	4		8.71
Cytidine	4-Amino-1-β-D-ribofuranosyl-2(1H)-pyrimidinone	C ₉ H ₁₃ N ₃ O ₅	65-46-3	243.216	1		4.22
Cytidine	4-Amino-1-β-D-ribofuranosyl-2(1H)-pyrimidinone	C ₉ H ₁₃ N ₃ O ₅	65-46-3	243.216	2		12.5
3'-Cytidylic acid	Cytidine 3'-monophosphate	C ₉ H ₁₄ N ₃ O ₈ P	84-52-6	323.196	1		0.8
3'-Cytidylic acid	Cytidine 3'-monophosphate	C ₉ H ₁₄ N ₃ O ₈ P	84-52-6	323.196	2		4.28
3'-Cytidylic acid	Cytidine 3'-monophosphate	C ₉ H ₁₄ N ₃ O ₈ P	84-52-6	323.196	3		6.0
Cytisine	Sophorine	C ₁₁ H ₁₄ N ₂ O	485-35-8	190.241	1		6.11
Cytisine	Sophorine	C ₁₁ H ₁₄ N ₂ O	485-35-8	190.241	2		13.08
Cytosine		C ₄ H ₅ N ₃ O	71-30-7	111.102	1		4.60
Cytosine		C ₄ H ₅ N ₃ O	71-30-7	111.102	2		12.16
Decylamine	1-Decanamine	C ₁₀ H ₂₃ N	2016-57-1	157.297		25	10.64
D-2-Deoxyribose		C ₅ H ₁₀ O ₄	533-67-5	134.131		25	12.61
2,4-Diaminobutanoic acid		C ₄ H ₁₀ N ₂ O ₂	305-62-4	118.134	1	25	1.85
2,4-Diaminobutanoic acid		C ₄ H ₁₀ N ₂ O ₂	305-62-4	118.134	2	25	8.24
2,4-Diaminobutanoic acid		C ₄ H ₁₀ N ₂ O ₂	305-62-4	118.134	3	25	10.44
1,3-Diamino-2-propanol		C ₃ H ₁₀ N ₂ O	616-29-5	90.123	1	20	9.69
1,3-Diamino-2-propanol		C ₃ H ₁₀ N ₂ O	616-29-5	90.123	2	20	7.93
Dibenzepin		C ₁₈ H ₂₁ N ₃ O	4498-32-2	295.379			8.25
3,5-Dibromoaniline		C ₆ H ₃ Br ₂ N	626-40-4	250.919		25	2.34
3,5-Dibromo-4-hydroxybenzotrile	Bromoxynil	C ₇ H ₃ Br ₂ NO	1689-84-5	276.913			4.06
3,5-Dibromo-L-tyrosine		C ₉ H ₉ Br ₂ NO ₃	300-38-9	338.980	1		2.17
3,5-Dibromo-L-tyrosine		C ₉ H ₉ Br ₂ NO ₃	300-38-9	338.980	2		6.45
3,5-Dibromo-L-tyrosine		C ₉ H ₉ Br ₂ NO ₃	300-38-9	338.980	3		7.60
Dibutylamine	N-Butylbutanamine	C ₈ H ₁₉ N	111-92-2	129.244		21	11.25
2,6-Di-tert-butylpyridine		C ₁₃ H ₂₁ N	585-48-8	191.313			3.58
Dichloroacetic acid		C ₂ H ₂ Cl ₂ O ₂	79-43-6	128.942		25	1.35
2,4-Dichloroaniline		C ₆ H ₃ Cl ₂ N	554-00-7	162.017		22	2.05
2,3-Dichlorophenol		C ₆ H ₄ Cl ₂ O	576-24-9	163.001		25	7.44
Dicyclohexylamine	N-Cyclohexylcyclohexanamine	C ₁₂ H ₂₃ N	101-83-7	181.318			10.4
2',3'-Dideoxyinosine	Didanosine	C ₁₀ H ₁₂ N ₄ O ₃	69655-05-6	236.227			9.12
Diethylamine	N-Ethylethanamine	C ₄ H ₁₁ N	109-89-7	73.137		25	10.84
N,N-Diethylaniline		C ₁₀ H ₁₅ N	91-66-7	149.233		25	6.57
Diethylmethylamine	N-Ethyl-N-methylethanamine	C ₅ H ₁₃ N	616-39-7	87.164		25	10.35
N,N-Diethyl-2-methylaniline		C ₁₁ H ₁₇ N	606-46-2	163.260		25	7.24
1,7-Dihydro-6H-purine-6-thione	6-Mercaptopurine	C ₅ H ₄ N ₄ S	50-44-2	152.178	1		7.77
1,7-Dihydro-6H-purine-6-thione	6-Mercaptopurine	C ₅ H ₄ N ₄ S	50-44-2	152.178	2		11.17
2,5-Dihydroxybenzeneacetic acid	Homogentisic acid	C ₈ H ₈ O ₄	451-13-8	168.148		25	4.40
2,4-Dihydroxybenzoic acid	β-Resorcylic acid	C ₇ H ₆ O ₄	89-86-1	154.121	1	25	3.11
2,4-Dihydroxybenzoic acid	β-Resorcylic acid	C ₇ H ₆ O ₄	89-86-1	154.121	2	25	8.55
2,4-Dihydroxybenzoic acid	β-Resorcylic acid	C ₇ H ₆ O ₄	89-86-1	154.121	3	25	14.0
2,5-Dihydroxybenzoic acid	Gentisic acid	C ₇ H ₆ O ₄	490-79-9	154.121	1	25	2.97
3,4-Dihydroxybenzoic acid	Protocatechuic acid	C ₇ H ₆ O ₄	99-50-3	154.121	1	25	4.48

3,4-Dihydroxybenzoic acid	Protocatechuic acid	C ₇ H ₆ O ₄	99-50-3	154.121	2	25	8.83
3,4-Dihydroxybenzoic acid	Protocatechuic acid	C ₇ H ₆ O ₄	99-50-3	154.121	3	25	12.6
3,5-Dihydroxybenzoic acid		C ₇ H ₆ O ₄	99-10-5	154.121	1	25	4.04
3,1,2-Dihydroxycholan-24-oic acid, (3 α ,5 β ,12 α)	Deoxycholic acid	C ₂₄ H ₄₀ O ₄	83-44-3	392.573			6.58
Dihydroxytartaric acid		C ₄ H ₆ O ₈	76-30-2	182.086		25	1.92
3,5-Diiodo- <i>L</i> -tyrosine		C ₉ H ₉ I ₂ NO ₃	300-39-0	432.981	1	25	2.12
3,5-Diiodo- <i>L</i> -tyrosine		C ₉ H ₉ I ₂ NO ₃	300-39-0	432.981	2	25	5.32
3,5-Diiodo- <i>L</i> -tyrosine		C ₉ H ₉ I ₂ NO ₃	300-39-0	432.981	3	25	9.48
Diisopropylamine	<i>N</i> -Isopropyl-2-propanamine	C ₆ H ₁₃ N	108-18-9	101.190		25	11.05
Dimethylamine	<i>N</i> -Methylmethanamine	C ₂ H ₇ N	124-40-3	45.084		25	10.73
4-(Dimethylamino)benzoic acid		C ₉ H ₁₁ NO ₂	619-84-1	165.189	1		6.03
4-(Dimethylamino)benzoic acid		C ₉ H ₁₁ NO ₂	619-84-1	165.189	2		11.49
2-Dimethylaminopurine	<i>N,N</i> -Dimethyl-1 <i>H</i> -purin-6-amine	C ₇ H ₈ N ₅	938-55-6	163.180	1	20	4.00
2-Dimethylaminopurine	<i>N,N</i> -Dimethyl-1 <i>H</i> -purin-6-amine	C ₇ H ₈ N ₅	938-55-6	163.180	2	20	10.24
2,6-Dimethylaniline	2,6-Xylidine	C ₈ H ₁₁ N	87-62-7	121.180		25	3.89
<i>N,N</i> -Dimethylaniline		C ₈ H ₁₁ N	121-69-7	121.180		25	5.07
Dimethylarsinic acid	Cacodylic acid	C ₂ H ₇ AsO ₂	75-60-5	137.998	1	25	1.57
Dimethylarsinic acid	Cacodylic acid	C ₂ H ₇ AsO ₂	75-60-5	137.998	2	25	6.27
3,5-Dimethylbenzoic acid	Mesitylenic acid	C ₉ H ₁₀ O ₂	499-06-9	150.174		25	4.32
5,5-Dimethyl-1,3-cyclohexanedione	5,5-Dimethylidihydroresorcinol	C ₈ H ₁₂ O ₂	126-81-8	140.180		25	5.15
2,2-Dimethyl-1,3-dioxane-4,6-dione	Meldrum's acid	C ₆ H ₈ O ₄	2033-24-1	144.126			5.1
<i>N,N</i> -Dimethylglycine		C ₄ H ₉ NO ₂	1118-68-9	103.120		25	9.89
2,4-Dimethyl-1 <i>H</i> -imidazole		C ₅ H ₈ N ₂	930-62-1	96.131		25	8.36
Dimethylmalonic acid	Dimethylpropanedioic acid	C ₆ H ₈ O ₄	595-46-0	132.116		25	3.15
<i>N,N</i> -Dimethyl-1-naphthylamine		C ₁₂ H ₁₃ N	86-56-6	171.238		25	4.83
<i>N,N</i> -Dimethyl-2-naphthylamine		C ₁₂ H ₁₃ N	2436-85-3	171.238		25	4.566
<i>N,N</i> -Dimethyl-3-nitroaniline		C ₈ H ₁₀ N ₂ O ₂	619-31-8	166.177		25	2.62
5,5-Dimethyl-2,4-oxazolinedione	Dimethadione	C ₆ H ₇ NO ₃	695-53-4	129.115		37	6.13
<i>cis</i> -2,5-Dimethylpiperazine		C ₆ H ₁₄ N ₂	6284-84-0	114.188	1	25	9.66
<i>cis</i> -2,5-Dimethylpiperazine		C ₆ H ₁₄ N ₂	6284-84-0	114.188	2	25	5.20
1,2-Dimethylpiperidine, (\pm)-		C ₇ H ₁₅ N	2512-81-4	113.201		25	10.22
2,2-Dimethylpropanoic acid	Trimethylacetic acid	C ₅ H ₁₀ O ₂	75-98-9	102.132		20	5.03
2,2-Dimethylpropylamine	2,2-Dimethyl-1-propanamine	C ₅ H ₁₃ N	5813-64-9	87.164		25	10.15
2,3-Dimethylpyridine	2,3-Lutidine	C ₇ H ₉ N	583-61-9	107.153		25	6.57
2,4-Dimethylpyridine	2,4-Lutidine	C ₇ H ₉ N	108-47-4	107.153		25	6.99
2,5-Dimethylpyridine	2,5-Lutidine	C ₇ H ₉ N	589-93-5	107.153		25	6.40
2,6-Dimethylpyridine	2,6-Lutidine	C ₇ H ₉ N	108-48-5	107.153		25	6.65
3,4-Dimethylpyridine	3,4-Lutidine	C ₇ H ₉ N	583-58-4	107.153		25	6.46
3,5-Dimethylpyridine	3,5-Lutidine	C ₇ H ₉ N	591-22-0	107.153		25	6.15
4,6-Dimethyl-2-pyrimidinamine		C ₆ H ₉ N ₃	767-15-7	123.155		20	4.82
1,2-Dimethylpyrrolidine		C ₆ H ₁₃ N	765-48-0	99.174		26	10.20
2,4-Dinitrobenzoic acid		C ₇ H ₄ N ₂ O ₆	610-30-0	212.116		25	1.43
2,4-Dinitrophenol		C ₆ H ₄ N ₂ O ₅	51-28-5	184.106		25	4.07
2,5-Dinitrophenol		C ₆ H ₄ N ₂ O ₅	329-71-5	184.106		15	5.15
Dinoseb	Phenol, 2-(1-methylpropyl)-4,6-dinitro-	C ₁₀ H ₁₂ N ₂ O ₅	88-85-7	240.212			4.62
Diphenylamine	<i>N</i> -Phenylbenzenamine	C ₁₂ H ₁₁ N	122-39-4	169.222		25	0.79
4-[(Dipropylamino)sulfonyl]benzoic acid	Probenecid	C ₁₃ H ₁₉ NO ₄ S	57-66-9	285.360			5.8
Dodecylamine	1-Dodecanamine	C ₁₂ H ₂₇ N	124-22-1	185.349		25	10.63
Dopamine	4(2-Aminoethyl)-1,2-benzenediol	C ₈ H ₁₁ NO ₂	51-61-6	153.179	1	25	8.9
Dopamine	4(2-Aminoethyl)-1,2-benzenediol	C ₈ H ₁₁ NO ₂	51-61-6	153.179	2	25	10.6
Droperidol	Dehydrobenzperidol	C ₂₂ H ₂₂ FN ₃ O ₂	548-73-2	379.427			7.64
Emetine	6',7',10,11-Tetramethoxyemetan	C ₂₉ H ₄₀ N ₂ O ₄	483-18-1	480.639	1		5.77
Emetine	6',7',10,11-Tetramethoxyemetan	C ₂₉ H ₄₀ N ₂ O ₄	483-18-1	480.639	2		6.64
<i>d</i> -Ephedrine	α -[1-(Methylamino)ethyl]benzenemethanol, [5-(<i>R</i> *, <i>S</i> *)]-	C ₁₀ H ₁₅ NO	321-98-2	165.232		10	10.139
<i>l</i> -Ephedrine	α -[1-(Methylamino)ethyl]benzenemethanol, [1 <i>R</i> -(<i>R</i> *, <i>S</i> *)]-	C ₁₀ H ₁₅ NO	299-42-3	165.232		10	9.958
Epinephrine	<i>D</i> -Adrenaline	C ₈ H ₁₃ NO ₃	51-43-4	183.204	1	25	8.66
Epinephrine	<i>D</i> -Adrenaline	C ₈ H ₁₃ NO ₃	51-43-4	183.204	2	25	9.95
Ergometrinine		C ₁₉ H ₂₃ N ₃ O ₂	479-00-5	325.405			7.3
Ergonovine	Ergometrine	C ₁₉ H ₂₃ N ₃ O ₂	60-79-7	325.405			6.8

Erythromycin	Propioline	C ₂₇ H ₄₇ NO ₁₃	114-07-8	733.927			8.8
Ethacrynic acid	[2,3-Dichloro-4-(2-methylene-1-oxobutyl)phenoxy]acetic acid	C ₁₃ H ₁₂ Cl ₂ O ₄	58-54-8	303.138			3.50
1,2-Ethanediamine	Ethylenediamine	C ₂ H ₈ N ₂	107-15-3	60.098	1	25	9.92
1,2-Ethanediamine	Ethylenediamine	C ₂ H ₈ N ₂	107-15-3	60.098	2	25	6.86
1,2-Ethandiol	Ethylene glycol	C ₂ H ₆ O ₂	107-21-1	62.068		25	15.1
Ethanimidamide		C ₂ H ₆ N ₂	143-37-3	58.082		25	12.1
Ethanol	Ethyl alcohol	C ₂ H ₆ O	64-17-5	46.068		25	15.5
Ethanolamine	Glycinol	C ₂ H ₇ NO	141-43-5	61.083		25	9.50
Ethoxyacetic acid		C ₄ H ₈ O ₃	627-03-2	104.105		18	3.65
2-Ethoxyaniline	<i>o</i> -Phenetidine	C ₈ H ₁₁ NO	94-70-2	137.179		28	4.43
3-Ethoxyaniline	<i>m</i> -Phenetidine	C ₈ H ₁₁ NO	621-33-0	137.179		25	4.18
4-Ethoxyaniline	<i>p</i> -Phenetidine	C ₈ H ₁₁ NO	156-43-4	137.179		28	5.20
Ethyl acetoacetate		C ₈ H ₁₀ O ₃	141-97-9	130.141		25	10.68
Ethylamine	Ethanamine	C ₂ H ₇ N	75-04-7	45.084		25	10.65
Ethyl 4-aminobenzoate	Benzocaine	C ₉ H ₁₁ NO ₂	94-09-7	165.189			2.5
<i>N</i> -Ethylaniline		C ₈ H ₁₁ N	103-69-5	121.180		25	5.12
2-Ethyl-1 <i>H</i> -benzimidazole		C ₉ H ₁₀ N ₂	1848-84-6	146.188		25	6.18
<i>O</i> -Ethyl S-[2-(diisopropylamino)ethyl] methylphosphonothioate	VX Nerve agent	C ₁₁ H ₂₆ NO ₂ PS	50782-69-9	267.369			7.9
Ethyleneimine	Aziridine	C ₂ H ₅ N	151-56-4	43.068		25	8.04
α -Ethylglutamic acid		C ₇ H ₁₃ NO ₄	20913-68-2	175.183	1	25	3.846
α -Ethylglutamic acid		C ₇ H ₁₃ NO ₄	20913-68-2	175.183	2	25	7.838
<i>N</i> -Ethylmorpholine		C ₆ H ₁₃ NO	100-74-3	115.173		25	7.67
1-Ethylpiperidine		C ₇ H ₁₃ N	766-09-6	113.201		23	10.45
2-Ethylpyridine		C ₇ H ₉ N	100-71-0	107.153		25	5.89
Etoposide		C ₂₉ H ₃₂ O ₁₃	33419-42-0	588.556			9.8
Fluoroacetic acid	Fluoroethanoic acid	C ₂ H ₃ FO ₂	144-49-0	78.042		25	2.59
2-Fluoroaniline		C ₆ H ₆ FN	348-54-9	111.117		25	3.20
3-Fluoroaniline		C ₆ H ₆ FN	372-19-0	111.117		25	3.59
4-Fluoroaniline		C ₆ H ₆ FN	371-40-4	111.117		25	4.65
2-Fluorobenzoic acid		C ₇ H ₅ FO ₂	445-29-4	140.112		25	3.27
3-Fluorobenzoic acid		C ₇ H ₅ FO ₂	455-38-9	140.112		25	3.86
4-Fluorobenzoic acid		C ₇ H ₅ FO ₂	456-22-4	140.112		25	4.15
5-Fluorocytosine	4-Amino-5-fluoro-2-hydroxypyrimidine	C ₄ H ₄ FN ₃ O	2022-85-7	129.092			3.26
2-Fluorophenol		C ₆ H ₅ FO	367-12-4	112.101		25	8.73
3-Fluorophenol		C ₆ H ₅ FO	372-20-3	112.101		25	9.29
4-Fluorophenol		C ₆ H ₅ FO	371-41-5	112.101		25	9.89
2-Fluoropyridine		C ₅ H ₄ FN	372-48-5	97.091		25	-0.44
Folic acid	5-Formyl-5,6,7,8-tetrahydrofolic acid	C ₂₀ H ₂₃ N ₇ O ₇	58-05-9	473.440	1		3.1
Folic acid	5-Formyl-5,6,7,8-tetrahydrofolic acid	C ₂₀ H ₂₃ N ₇ O ₇	58-05-9	473.440	2		4.8
Folic acid	5-Formyl-5,6,7,8-tetrahydrofolic acid	C ₂₀ H ₂₃ N ₇ O ₇	58-05-9	473.440	3		10.4
Formaldehyde	Methanal	CH ₂ O	50-00-0	30.026		25	13.27
Formic acid	Methanoic acid	CH ₂ O ₂	64-18-6	46.026		25	3.75
3-Formylbenzoic acid		C ₈ H ₆ O ₃	619-21-6	150.132		25	3.84
4-Formylbenzoic acid		C ₈ H ₆ O ₃	619-66-9	150.132		25	3.77
β - <i>D</i> -Fructose	β -Levulose	C ₆ H ₁₂ O ₆	53188-23-1	180.155		25	12.27
Fumaric acid	<i>trans</i> -2-Butenedioic acid	C ₄ H ₄ O ₄	110-17-8	116.073	1	25	3.02
Fumaric acid	<i>trans</i> -2-Butenedioic acid	C ₄ H ₄ O ₄	110-17-8	116.073	2	25	4.38
2-Furancarboxylic acid	2-Furoic acid	C ₅ H ₄ O ₃	88-14-2	112.084		25	3.16
3-Furancarboxylic acid		C ₅ H ₄ O ₃	488-93-7	112.084		25	3.9
Furethidine		C ₂₁ H ₃₁ NO ₄	2385-81-1	361.476			7.48
Gibberellic acid		C ₁₉ H ₃₂ O ₆	77-06-5	346.374			4.0
α - <i>D</i> -Glucose		C ₆ H ₁₂ O ₆	26655-34-5	180.155		25	12.46
<i>L</i> -Glutamic acid	(<i>S</i>)-2-Aminopentanedioic acid	C ₅ H ₉ NO ₄	56-86-0	147.130	1	25	2.13
<i>L</i> -Glutamic acid	(<i>S</i>)-2-Aminopentanedioic acid	C ₅ H ₉ NO ₄	56-86-0	147.130	2	25	4.31
<i>L</i> -Glutamic acid	(<i>S</i>)-2-Aminopentanedioic acid	C ₅ H ₉ NO ₄	56-86-0	147.130	3		9.67
<i>L</i> -Glutamine	2-Aminoglutaric acid	C ₅ H ₁₀ N ₂ O ₃	56-85-9	146.144	1	25	2.17
<i>L</i> -Glutamine	2-Aminoglutaric acid	C ₅ H ₁₀ N ₂ O ₃	56-85-9	146.144	2	25	9.13

Glutathione	<i>L</i> -γ-Glutamyl- <i>L</i> -cysteinylglycine	C ₁₀ H ₁₇ N ₃ O ₆ S	70-18-8	307.323	1	25	2.12
Glutathione	<i>L</i> -γ-Glutamyl- <i>L</i> -cysteinylglycine	C ₁₀ H ₁₇ N ₃ O ₆ S	70-18-8	307.323	2	25	3.59
Glutathione	<i>L</i> -γ-Glutamyl- <i>L</i> -cysteinylglycine	C ₁₀ H ₁₇ N ₃ O ₆ S	70-18-8	307.323	3	25	8.75
Glutathione	<i>L</i> -γ-Glutamyl- <i>L</i> -cysteinylglycine	C ₁₀ H ₁₇ N ₃ O ₆ S	70-18-8	307.323	4	25	9.65
Glyceric acid		C ₃ H ₆ O ₄	473-81-4	106.078		25	3.52
Glycerol	1,2,3-Propanetriol	C ₃ H ₈ O ₃	56-81-5	92.094		25	14.15
Glycine	Aminoacetic acid	C ₂ H ₅ NO ₂	56-40-6	75.067	1	25	2.35
Glycine	Aminoacetic acid	C ₂ H ₅ NO ₂	56-40-6	75.067	2	25	9.78
Glycocholic acid	<i>N</i> -(3,7,12-Trihydroxy-24-oxochola <i>N</i> (24-yl)glycine, (3α,5β,7α,12α)	C ₂₆ H ₄₃ NO ₆	475-31-0	465.622			4.4
Glycolic acid		C ₂ H ₄ O ₃	79-14-1	76.051		25	3.83
Glycylalanine	<i>N</i> -Alanylglycine	C ₈ H ₁₀ N ₂ O ₃	1188-01-8	146.144		25	3.15
<i>L</i> -Glycylasparagine		C ₆ H ₁₁ N ₃ O ₄	1999-33-3	189.169	1	25	2.942
<i>L</i> -Glycylasparagine		C ₆ H ₁₁ N ₃ O ₄	1999-33-3	189.169	2	18	8.44
<i>N</i> -Glycylglycine	2-(Aminoacetamido)acetic acid	C ₄ H ₈ N ₂ O ₃	556-50-3	132.118	1	25	3.14
<i>N</i> -Glycylglycine	2-(Aminoacetamido)acetic acid	C ₄ H ₈ N ₂ O ₃	556-50-3	132.118	2		8.17
<i>N</i> -(<i>N</i> -Glycylglycyl)glycine		C ₆ H ₁₁ N ₃ O ₄	556-33-2	189.169	1	25	3.225
<i>N</i> -(<i>N</i> -Glycylglycyl)glycine		C ₆ H ₁₁ N ₃ O ₄	556-33-2	189.169	2	25	8.09
<i>N</i> -Glycyl- <i>L</i> -leucine		C ₈ H ₁₆ N ₂ O ₃	869-19-2	188.224		25	3.18
<i>N</i> -Glycylserine, (<i>DL</i>)-		C ₅ H ₁₀ N ₂ O ₄	687-38-7	162.144	1	25	2.98
<i>N</i> -Glycylserine, (<i>DL</i>)-		C ₅ H ₁₀ N ₂ O ₄	687-38-7	162.144	2	25	8.38
Glyoxylic acid		C ₂ H ₂ O ₃	298-12-4	74.035		25	3.18
Guanidine	Aminomethanamide	CH ₅ N ₃	113-00-8	59.071		25	13.6
Guanidinoacetic acid	Glycoxyamine	C ₃ H ₇ N ₃ O ₂	352-97-6	117.107		25	2.82
Guanine		C ₅ H ₅ N ₅ O	73-40-5	151.127		40	9.92
Haloperidol		C ₂₁ H ₂₃ ClFNO ₂	52-86-8	375.865			8.3
Harmaline	4,9-Dihydro-7-methoxy-1-methyl-3 <i>H</i> -pyrido[3,4- <i>b</i>]indole	C ₁₃ H ₁₄ N ₂ O	304-21-2	214.262			4.2
Harmine	7-Methoxy-1-methyl-9 <i>H</i> -pyrido[3,4- <i>b</i>]indole	C ₁₃ H ₁₂ N ₂ O	442-51-3	212.246			7.70
2-Heptanamine	Tuaminoheptane	C ₇ H ₁₇ N	123-82-0	115.217		19	10.7
Heptanedioic acid	Pimelic acid	C ₇ H ₁₂ O ₄	111-16-0	160.168	1	25	4.71
Heptanedioic acid	Pimelic acid	C ₇ H ₁₂ O ₄	111-16-0	160.168	2	25	5.58
Heptanoic acid	Enanthic acid	C ₇ H ₁₄ O ₂	111-14-8	130.185		25	4.89
Heptylamine	1-Heptanamine	C ₇ H ₁₇ N	111-68-2	115.217		25	10.67
Hexadecylamine	1-Hexadecanamine	C ₁₆ H ₃₃ N	143-27-1	241.456		25	10.61
2,4-Hexadienoic acid	Sorbic acid	C ₆ H ₈ O ₂	110-44-1	112.127		25	4.76
Hexamethyldisilazane		C ₆ H ₁₉ NSi ₂	999-97-3	161.393			7.55
1,6-Hexanediamine	Hexamethylenediamine	C ₆ H ₁₆ N ₂	124-09-4	116.204	1	0	11.86
1,6-Hexanediamine	Hexamethylenediamine	C ₆ H ₁₆ N ₂	124-09-4	116.204	2	0	10.76
1,6-Hexanedioic acid	Adipic acid	C ₆ H ₁₀ O ₄	124-04-9	146.141	1	18	4.41
1,6-Hexanedioic acid	Adipic acid	C ₆ H ₁₀ O ₄	124-04-9	146.141	2	18	5.41
Hexanoic acid	Caproic acid	C ₆ H ₁₂ O ₂	142-62-1	116.158		25	4.85
Hexylamine	1-Hexanamine	C ₆ H ₁₅ N	111-26-2	101.190		25	10.56
Histamine		C ₅ H ₉ N ₃	51-45-6	111.145	1	25	6.04
Histamine		C ₅ H ₉ N ₃	51-45-6	111.145	2	25	9.75
<i>L</i> -Histidine	Glyoxaline-5-alanine	C ₆ H ₉ N ₃ O ₂	71-00-1	155.154	1	25	1.80
<i>L</i> -Histidine	Glyoxaline-5-alanine	C ₆ H ₉ N ₃ O ₂	71-00-1	155.154	2	25	6.04
<i>L</i> -Histidine	Glyoxaline-5-alanine	C ₆ H ₉ N ₃ O ₂	71-00-1	155.154	3	25	9.33
<i>DL</i> -Homocysteine	<i>DL</i> -2-Amino-4-mercaptobutanoic acid	C ₄ H ₉ NO ₂ S	454-29-5	135.185	1	25	2.22
<i>DL</i> -Homocysteine	<i>DL</i> -2-Amino-4-mercaptobutanoic acid	C ₄ H ₉ NO ₂ S	454-29-5	135.185	2	25	8.87
<i>DL</i> -Homocysteine	<i>DL</i> -2-Amino-4-mercaptobutanoic acid	C ₄ H ₉ NO ₂ S	454-29-5	135.185	3	25	10.86
Homocystine		C ₈ H ₁₆ N ₂ O ₄ S ₂	870-93-9	268.354	1	25	1.59
Homocystine		C ₈ H ₁₆ N ₂ O ₄ S ₂	870-93-9	268.354	2	25	2.54
Homocystine		C ₈ H ₁₆ N ₂ O ₄ S ₂	870-93-9	268.354	3	25	8.52
Homocystine		C ₈ H ₁₆ N ₂ O ₄ S ₂	870-93-9	268.354	4	25	9.44
<i>L</i> -Homoserine	2-Amino-4-hydroxybutanoic acid, (5)-	C ₄ H ₉ NO ₃	672-15-1	119.119	1	25	2.71
<i>L</i> -Homoserine	2-Amino-4-hydroxybutanoic acid, (5)-	C ₄ H ₉ NO ₃	672-15-1	119.119	2	25	9.62
Hydrastine		C ₂₁ H ₂₁ NO ₆	118-08-1	383.395			7.8
Hydrastinine	5,6,7,8-Tetrahydro-6-methyl-1,3-dioxolo[4,5- <i>g</i>]isoquinolin-5-ol	C ₁₁ H ₁₃ NO ₃	6592-85-4	207.226			11.38

Hydrochlorothiazide		C ₇ H ₈ ClN ₃ O ₄ S ₂	58-93-5	297.740	1		7.9
Hydrochlorothiazide		C ₇ H ₈ ClN ₃ O ₄ S ₂	58-93-5	297.740	2		9.2
Hydroflumethiazide		C ₈ H ₈ F ₃ N ₃ O ₄ S ₂	135-09-1	331.293	1		8.9
Hydroflumethiazide		C ₈ H ₈ F ₃ N ₃ O ₄ S ₂	135-09-1	331.293	2		9.7
Hydroquinine		C ₂₀ H ₂₆ N ₂ O ₂	522-66-7	326.432			5.33
<i>p</i> -Hydroquinone	1,4-Benzenediol	C ₆ H ₆ O ₂	123-31-9	110.111	1	25	9.85
<i>p</i> -Hydroquinone	1,4-Benzenediol	C ₆ H ₆ O ₂	123-31-9	110.111	2	25	11.4
3-Hydroxybenzaldehyde	3-Formylphenol	C ₇ H ₆ O ₂	100-83-4	122.122		25	8.98
4-Hydroxybenzaldehyde	4-Formylphenol	C ₇ H ₆ O ₂	123-08-0	122.122		25	7.61
α -Hydroxybenzeneacetic acid, (\pm)-	<i>DL</i> -Mandelic acid	C ₈ H ₈ O ₃	611-72-3	152.148		25	3.37
3-Hydroxybenzenesulfonic acid	<i>m</i> -Phenolsulfonic acid	C ₆ H ₆ O ₃ S	585-38-6	174.175		25	9.07
4-Hydroxybenzenesulfonic acid	<i>p</i> -Phenolsulfonic acid	C ₆ H ₆ O ₃ S	98-67-9	174.175		25	9.11
2-Hydroxybenzoic acid	Salicylic acid	C ₇ H ₆ O ₃	69-72-7	138.121	1	20	2.98
2-Hydroxybenzoic acid	Salicylic acid	C ₇ H ₆ O ₃	69-72-7	138.121	2	20	13.6
3-Hydroxybenzoic acid		C ₇ H ₆ O ₃	99-06-9	138.121	1	25	4.08
3-Hydroxybenzoic acid		C ₇ H ₆ O ₃	99-06-9	138.121	2	19	9.92
4-Hydroxybenzoic acid		C ₇ H ₆ O ₃	99-96-7	138.121	1	25	4.57
4-Hydroxybenzoic acid		C ₇ H ₆ O ₃	99-96-7	138.121	2	25	9.46
2-Hydroxybenzotrile		C ₇ H ₅ NO	611-20-1	119.121		25	6.86
3-Hydroxybenzotrile		C ₇ H ₅ NO	873-62-1	119.121		25	8.61
4-Hydroxybenzotrile		C ₇ H ₅ NO	767-00-0	119.121		25	7.97
2-Hydroxybiphenyl	[1,1'-Biphenyl]-2-ol	C ₁₂ H ₁₀ O	90-43-7	170.206		25	10.01
3-Hydroxybiphenyl	[1,1'-Biphenyl]-3-ol	C ₁₂ H ₁₀ O	580-51-8	170.206		25	9.64
4-Hydroxybiphenyl	[1,1'-Biphenyl]-4-ol	C ₁₂ H ₁₀ O	92-69-3	170.206		25	9.55
3-Hydroxybutanoic acid, (\pm)-		C ₄ H ₈ O ₃	625-71-8	104.105		25	4.70
4-Hydroxybutanoic acid		C ₄ H ₈ O ₃	591-81-1	104.105		25	4.72
1-Hydroxy-1,1-diphosphonoethane	Etidronic acid	C ₂ H ₈ O ₇ P ₂	2809-21-4	206.028	1		1.35
1-Hydroxy-1,1-diphosphonoethane	Etidronic acid	C ₂ H ₈ O ₇ P ₂	2809-21-4	206.028	2		2.87
1-Hydroxy-1,1-diphosphonoethane	Etidronic acid	C ₂ H ₈ O ₇ P ₂	2809-21-4	206.028	3		7.03
1-Hydroxy-1,1-diphosphonoethane	Etidronic acid	C ₂ H ₈ O ₇ P ₂	2809-21-4	206.028	4		11.3
5-Hydroxy-2-(hydroxymethyl)-4 <i>H</i> -pyran-4-one	Kojic acid	C ₆ H ₆ O ₄	501-30-4	142.110			7.9
α -Hydroxy- α -methylbenzeneacetic acid	Atrolactic acid	C ₉ H ₁₀ O ₃	515-30-0	166.173		25	3.47
α -Hydroxy- α -phenylbenzeneacetic acid	Benzilic acid	C ₁₁ H ₁₂ O ₃	76-93-7	228.243		25	3.04
1-(2-Hydroxyphenyl)ethanone	2-Hydroxyacetophenone	C ₈ H ₈ O ₂	118-93-4	136.149		25	10.06
1-(3-Hydroxyphenyl)ethanone	3-Hydroxyacetophenone	C ₈ H ₈ O ₂	121-71-1	136.149		25	9.19
1-(4-Hydroxyphenyl)ethanone	4-Hydroxyacetophenone	C ₈ H ₈ O ₂	99-93-4	136.149		25	8.05
<i>trans</i> -4-Hydroxy- <i>L</i> -proline		C ₅ H ₉ NO ₃	51-35-4	131.130	1	25	1.82
<i>trans</i> -4-Hydroxy- <i>L</i> -proline		C ₅ H ₉ NO ₃	51-35-4	131.130	2	25	9.66
Hydroxypropanedioic acid	Tartronic acid	C ₃ H ₄ O ₅	80-69-3	120.061	1		2.42
Hydroxypropanedioic acid	Tartronic acid	C ₃ H ₄ O ₅	80-69-3	120.061	2		4.54
3-Hydroxypropanoic acid	Hydracrylic acid	C ₃ H ₄ O ₃	503-66-2	90.078		25	4.51
5-Hydroxytryptamine	3-(2-Aminoethyl)indol-5-ol	C ₁₀ H ₁₂ N ₂ O	50-67-9	176.214	1	25	9.8
5-Hydroxytryptamine	3-(2-Aminoethyl)indol-5-ol	C ₁₀ H ₁₂ N ₂ O	50-67-9	176.214	2	25	11.1
Hyoscyamine		C ₁₇ H ₂₃ NO ₃	101-31-5	289.370		21	9.7
Hypoxanthine		C ₅ H ₄ N ₄ O	68-94-0	136.112		25	8.7
Imazapyr	2-(4-Isopropyl-4-methyl-5-oxo-2-imidazolin-2-yl)nicotinic acid	C ₁₃ H ₁₅ N ₃ O ₃	81334-34-1	261.276	1		1.9
Imazapyr	2-(4-Isopropyl-4-methyl-5-oxo-2-imidazolin-2-yl)nicotinic acid	C ₁₃ H ₁₅ N ₃ O ₃	81334-34-1	261.276	2		3.6
Imazethapyr	(<i>RS</i>)-5-Ethyl-2-(4-isopropyl-4-methyl-5-oxo-2-imidazolin-2-yl)nicotinic acid	C ₁₅ H ₁₉ N ₃ O ₃	81335-77-5	289.330	1		2.1
Imazethapyr	(<i>RS</i>)-5-Ethyl-2-(4-isopropyl-4-methyl-5-oxo-2-imidazolin-2-yl)nicotinic acid	C ₁₅ H ₁₉ N ₃ O ₃	81335-77-5	289.330	2		3.9
Imidazole	1,3-Diazole	C ₃ H ₄ N ₂	288-32-4	68.077		25	6.99
Iminodiacetic acid		C ₄ H ₇ NO ₄	142-73-4	133.104	1		2.98
Iminodiacetic acid		C ₄ H ₇ NO ₄	142-73-4	133.104	2		9.89
1-Indanamine	1-Aminoindane	C ₉ H ₁₁ N	34698-41-4	133.190		22	9.21

1 <i>H</i> -Indole-3-acetic acid	3-Indolylacetic acid	C ₁₀ H ₉ NO ₂	87-51-4	175.184			4.75
Indomethacin		C ₁₉ H ₁₆ ClNO ₄	53-86-1	357.788			4.5
Iocetamic acid		C ₁₂ H ₁₃ I ₃ N ₂ O ₃	16034-77-8	613.955			4
Iodoacetic acid		C ₂ H ₃ IO ₂	64-69-7	185.948		25	3.18
2-Iodoaniline		C ₆ H ₆ IN	615-43-0	219.023		25	2.54
3-Iodoaniline		C ₆ H ₆ IN	626-01-7	219.023		25	3.58
4-Iodoaniline		C ₆ H ₆ IN	540-37-4	219.023		25	3.81
2-Iodobenzoic acid		C ₇ H ₅ IO ₂	88-67-5	248.018		25	2.86
3-Iodobenzoic acid		C ₇ H ₅ IO ₂	618-51-9	248.018		25	3.87
4-Iodobenzoic acid		C ₇ H ₅ IO ₂	619-58-9	248.018		25	4.00
2-Iodophenol		C ₆ H ₅ IO	533-58-4	220.007		25	8.51
3-Iodophenol		C ₆ H ₅ IO	626-02-8	220.007		25	9.03
4-Iodophenol		C ₆ H ₅ IO	540-38-5	220.007		25	9.33
<i>L</i> -3-Iodotyrosine		C ₉ H ₁₀ INO ₃	70-78-0	307.084	1	25	2.2
<i>L</i> -3-Iodotyrosine		C ₉ H ₁₀ INO ₃	70-78-0	307.084	2	25	8.7
<i>L</i> -3-Iodotyrosine		C ₉ H ₁₀ INO ₃	70-78-0	307.084	3	25	9.1
Iopanoic acid		C ₁₁ H ₁₂ I ₂ NO ₂	96-83-3	570.932			4.8
Isocitric acid		C ₆ H ₈ O ₇	320-77-4	192.124	1	25	3.29
Isocitric acid		C ₆ H ₈ O ₇	320-77-4	192.124	2	25	4.71
Isocitric acid		C ₆ H ₈ O ₇	320-77-4	192.124	3	25	6.40
<i>L</i> -Isoleucine	2-Amino-3-methylpentanoic acid	C ₆ H ₁₃ NO ₂	73-32-5	131.173	1	25	2.32
<i>L</i> -Isoleucine	2-Amino-3-methylpentanoic acid	C ₆ H ₁₃ NO ₂	73-32-5	131.173	2	25	9.76
Isophthalic acid	1,3-Benzenedicarboxylic acid	C ₈ H ₆ O ₄	121-91-5	166.132	1	25	3.70
Isophthalic acid	1,3-Benzenedicarboxylic acid	C ₈ H ₆ O ₄	121-91-5	166.132	2	25	4.60
Isopropylamine	2-Propanamine	C ₃ H ₉ N	75-31-0	59.110		25	10.63
<i>N</i> -Isopropylamine		C ₆ H ₁₃ N	768-52-5	135.206		25	5.77
Isoproterenol	4-[1-Hydroxy-2-[isopropylamino]ethyl]-1,2-benzenediol	C ₁₁ H ₁₇ NO ₃	7683-59-2	211.258			8.64
1-Isoquinolinamine		C ₉ H ₈ N ₂	1532-84-9	144.173		20	7.62
3-Isoquinolinamine		C ₉ H ₈ N ₂	25475-67-6	144.173		20	5.05
Isoquinoline	Benzo[<i>c</i>]pyridine	C ₉ H ₇ N	119-65-3	129.159		20	5.40
7-Isoquinolinol		C ₉ H ₇ NO	7651-83-4	145.158	1	20	5.68
7-Isoquinolinol		C ₉ H ₇ NO	7651-83-4	145.158	2	20	8.90
Isoxazole	1-Oxa-2-azacyclopentadiene	C ₃ H ₃ NO	288-14-2	69.062		25	-2.0
Ketamine	2-(2-Chlorophenyl)-2-(methylamino)cyclohexanone, (±)-	C ₁₃ H ₁₆ ClNO	6740-88-1	237.725			7.5
<i>D</i> -Lactic acid	<i>D</i> -2-Hydroxypropanoic acid	C ₃ H ₆ O ₃	10326-41-7	90.078		25	3.86
<i>L</i> -Leucine	2-Amino-4-methylpentanoic acid	C ₆ H ₁₃ NO ₂	61-90-5	131.173	1	25	2.33
<i>L</i> -Leucine	2-Amino-4-methylpentanoic acid	C ₆ H ₁₃ NO ₂	61-90-5	131.173	2	25	9.74
<i>N</i> -Leucylglycine		C ₈ H ₁₆ N ₂ O ₃	686-50-0	188.224	1	25	3.25
<i>N</i> -Leucylglycine		C ₈ H ₁₆ N ₂ O ₃	686-50-0	188.224	2	25	8.2
Levodopa	<i>L</i> -3,4-Dihydroxyphenylalanine	C ₉ H ₁₁ NO ₄	59-92-7	197.188	1	25	2.32
Levodopa	<i>L</i> -3,4-Dihydroxyphenylalanine	C ₉ H ₁₁ NO ₄	59-92-7	197.188	2	25	8.72
Levodopa	<i>L</i> -3,4-Dihydroxyphenylalanine	C ₉ H ₁₁ NO ₄	59-92-7	197.188	3	25	9.96
Levodopa	<i>L</i> -3,4-Dihydroxyphenylalanine	C ₉ H ₁₁ NO ₄	59-92-7	197.188	4	25	11.79
Lisinopril		C ₂₁ H ₃₅ N ₃ O ₇	83915-83-7	441.519	1		2.5
Lisinopril		C ₂₁ H ₃₅ N ₃ O ₇	83915-83-7	441.519	2		4.0
Lisinopril		C ₂₁ H ₃₅ N ₃ O ₇	83915-83-7	441.519	3		6.7
Lisinopril		C ₂₁ H ₃₅ N ₃ O ₇	83915-83-7	441.519	4		10.1
Lycodine		C ₁₆ H ₂₂ N ₂	20316-18-1	242.359	1		3.97
Lycodine		C ₁₆ H ₂₂ N ₂	20316-18-1	242.359	2		8.08
Lysergic acid		C ₁₆ H ₁₆ N ₂ O ₂	82-58-6	268.310	1		3.44
Lysergic acid		C ₁₆ H ₁₆ N ₂ O ₂	82-58-6	268.310	2		7.68
<i>L</i> -Lysine	2,6-Diaminohexanoic acid, (<i>L</i> -)	C ₆ H ₁₄ N ₂ O ₂	56-87-1	146.187	1	25	2.16
<i>L</i> -Lysine	2,6-Diaminohexanoic acid, (<i>L</i> -)	C ₆ H ₁₄ N ₂ O ₂	56-87-1	146.187	2	25	9.06
<i>L</i> -Lysine	2,6-Diaminohexanoic acid, (<i>L</i> -)	C ₆ H ₁₄ N ₂ O ₂	56-87-1	146.187	3	25	10.54
Maleic acid	<i>cis</i> -2-Butenedioic acid	C ₄ H ₄ O ₄	110-16-7	116.073	1	25	1.92
Maleic acid	<i>cis</i> -2-Butenedioic acid	C ₄ H ₄ O ₄	110-16-7	116.073	2	25	6.23
Malic acid	Hydroxybutanedioic acid	C ₄ H ₆ O ₅	617-48-1	134.088	1	25	3.40
Malic acid	Hydroxybutanedioic acid	C ₄ H ₆ O ₅	617-48-1	134.088	2	25	5.11

Malonic acid		C ₃ H ₄ O ₄	141-82-2	104.062	1	25	2.85
Malonic acid		C ₃ H ₄ O ₄	141-82-2	104.062	2	25	5.70
α-Maltose		C ₁₂ H ₂₂ O ₁₁	4482-75-1	342.296		21	12.05
D-Mannitol	Cordycepic acid	C ₆ H ₁₄ O ₆	69-65-8	182.171		18	13.5
D-Mannose	Seminose	C ₆ H ₁₂ O ₆	3458-28-4	180.155		25	12.08
Mefenamic acid	2-[(2,3-Dimethylphenyl)amino]benzoic acid	C ₁₅ H ₁₅ NO ₂	61-68-7	241.286			4.2
Mefluidide		C ₁₁ H ₁₃ F ₃ N ₂ O ₃ S	53780-34-0	310.292			4.6
2-Mercaptoethanol		C ₂ H ₆ OS	60-24-2	78.133		25	9.72
Methanethiol	Methyl mercaptan	CH ₃ S	74-93-1	48.108		25	10.33
Methanol	Methyl alcohol	CH ₄ O	67-56-1	32.042		25	15.5
Metharbital	5,5-Diethyl-1-methyl-2,4,6(1 <i>H</i> ,3 <i>H</i> ,5 <i>H</i>)-pyrimidinetrione	C ₉ H ₁₄ N ₂ O ₃	50-11-3	198.218			8.45
Methazolamide		C ₅ H ₈ N ₄ O ₃ S ₂	554-57-4	236.273			7.30
L-Methionine		C ₅ H ₁₁ NO ₂ S	63-68-3	149.212	1	25	2.13
L-Methionine		C ₅ H ₁₁ NO ₂ S	63-68-3	149.212	2	25	9.27
Methoxamine hydrochloride		C ₁₁ H ₁₈ ClNO ₃	61-16-5	247.719		25	9.2
2-Methoxyaniline	<i>o</i> -Anisidine	C ₇ H ₉ NO	90-04-0	123.152		25	4.53
3-Methoxyaniline	<i>m</i> -Anisidine	C ₇ H ₉ NO	536-90-3	123.152		25	4.20
4-Methoxyaniline	<i>p</i> -Anisidine	C ₇ H ₉ NO	104-94-9	123.152		25	5.36
2-Methoxybenzoic acid		C ₈ H ₈ O ₃	579-75-9	152.148		25	4.08
3-Methoxybenzoic acid		C ₈ H ₈ O ₃	586-38-9	152.148		25	4.10
4-Methoxybenzoic acid	<i>p</i> -Anisic acid	C ₈ H ₈ O ₃	100-09-4	152.148		25	4.50
2-Methoxyethanol	Ethylene glycol monomethyl ether	C ₃ H ₈ O ₂	109-86-4	76.095		25	14.8
2-Methoxyethylamine	1-Amino-2-methoxyethane	C ₃ H ₉ NO	109-85-3	75.109		25	9.40
2-(2-Methoxyethyl)pyridine	Metyridine	C ₈ H ₁₁ NO	114-91-0	137.179			5.5
2-Methoxyphenol	Guaiacol	C ₇ H ₈ O ₂	90-05-1	124.138		25	9.98
3-Methoxyphenol		C ₇ H ₈ O ₂	150-19-6	124.138		25	9.65
4-Methoxyphenol		C ₇ H ₈ O ₂	150-76-5	124.138		25	10.21
2-Methoxypyridine		C ₆ H ₇ NO	1628-89-3	109.126		20	3.28
3-Methoxypyridine		C ₆ H ₇ NO	7295-76-3	109.126		25	4.78
4-Methoxypyridine		C ₆ H ₇ NO	620-08-6	109.126		25	6.58
6-Methoxyquinoline		C ₁₀ H ₉ NO	5263-87-6	159.184		20	5.03
Methclothiazide		C ₉ H ₁₁ Cl ₂ N ₃ O ₄ S ₂	135-07-9	360.237			9.4
2-Methylalanine	α-Aminoisobutyric acid	C ₄ H ₉ NO ₂	62-57-7	103.120	1	25	2.36
2-Methylalanine	α-Aminoisobutyric acid	C ₄ H ₉ NO ₂	62-57-7	103.120	2	25	10.21
Methylamine	Methanamine	CH ₅ N	74-89-5	31.058		25	10.66
2-(Methylamino)benzoic acid		C ₈ H ₉ NO ₂	119-68-6	151.163		25	5.34
3-(Methylamino)benzoic acid		C ₈ H ₉ NO ₂	51524-84-6	151.163		25	5.10
4-(Methylamino)benzoic acid		C ₈ H ₉ NO ₂	10541-83-0	151.163		25	5.04
2-Methylaniline	<i>o</i> -Toluidine	C ₇ H ₉ N	95-53-4	107.153		25	4.45
3-Methylaniline	<i>m</i> -Toluidine	C ₇ H ₉ N	108-44-1	107.153		25	4.71
4-Methylaniline	<i>p</i> -Toluidine	C ₇ H ₉ N	106-49-0	107.153		25	5.08
<i>N</i> -Methylaniline		C ₇ H ₉ N	100-61-8	107.153		25	4.85
α-Methylbenzeneacetic acid, (±)-		C ₉ H ₁₀ O ₂	2328-24-7	150.174		25	4.64
2-Methyl-1 <i>H</i> -benzimidazole		C ₈ H ₈ N ₂	615-15-6	132.163		25	6.19
3-Methyl-1-butanamine	Isopentylamine	C ₅ H ₁₃ N	107-85-7	87.164		25	10.60
2-Methyl-2-butanamine		C ₅ H ₁₃ N	594-39-8	87.164		19	10.85
2-Methylbutanoic acid	(±)-2-Methylbutyric acid	C ₆ H ₁₀ O ₂	600-07-7	102.132		25	4.80
3-Methylbutanoic acid	Isovaleric acid	C ₆ H ₁₀ O ₂	503-74-2	102.132		25	4.77
<i>trans</i> - <i>o</i> -Methylcinnamic acid		C ₁₀ H ₁₀ O ₂	2373-76-4	162.185		25	4.50
<i>trans</i> - <i>m</i> -Methylcinnamic acid		C ₁₀ H ₁₀ O ₂	3029-79-6	162.185		25	4.44
<i>trans</i> - <i>p</i> -Methylcinnamic acid		C ₁₀ H ₁₀ O ₂	1866-39-3	162.185		25	4.56
α-Methylenebenzeneacetic acid	Atropic acid	C ₉ H ₈ O ₂	492-38-6	148.159			4.35
Methyl α- <i>D</i> -glucopyranoside	α-Methylglucoside	C ₇ H ₁₄ O ₆	97-30-3	194.182		25	13.71
<i>N</i> -Methyl-2-heptanamine		C ₈ H ₁₉ N	540-43-2	129.244		17	10.99
<i>L</i> -1-Methylhistidine		C ₇ H ₁₁ N ₃ O ₂	332-80-9	169.181	1	25	1.69
<i>L</i> -1-Methylhistidine		C ₇ H ₁₁ N ₃ O ₂	332-80-9	169.181	2	25	6.48
<i>L</i> -1-Methylhistidine		C ₇ H ₁₁ N ₃ O ₂	332-80-9	169.181	3	25	8.85

L-3-Methylhistidine		C ₇ H ₁₁ N ₃ O ₂	368-16-1	169.181	1	25	1.92
L-3-Methylhistidine		C ₇ H ₁₁ N ₃ O ₂	368-16-1	169.181	2	25	6.56
L-3-Methylhistidine		C ₇ H ₁₁ N ₃ O ₂	368-16-1	169.181	3	25	8.73
O-Methylhydroxylamine	Methoxyamine	CH ₃ NO	67-62-9	47.057			12.5
1-Methylimidazol		C ₄ H ₆ N ₂	616-47-7	82.104		25	6.95
Methylmalonic acid		C ₄ H ₆ O ₄	516-05-2	118.089	1	25	3.07
Methylmalonic acid		C ₄ H ₆ O ₄	516-05-2	118.089	2	25	5.76
4-Methylmorpholine		C ₅ H ₁₁ NO	109-02-4	101.147		25	7.38
Methyl-1-naphthylamine	N-Methyl-1-naphthalenamine	C ₁₁ H ₁₁ N	2216-68-4	157.212		27	3.67
3-Methylpentanedioic acid	3-Methylglutaric acid	C ₆ H ₁₀ O ₄	626-51-7	146.141		25	4.24
4-Methylpentanoic acid		C ₆ H ₁₂ O ₂	646-07-1	116.158		18	4.84
Methylphenidate		C ₁₄ H ₁₉ NO ₂	113-45-1	233.307			8.9
1-Methylpiperidine		C ₆ H ₁₃ N	626-67-5	99.174		25	10.38
2-Methylpropanoic acid	Isobutyric acid	C ₄ H ₈ O ₂	79-31-2	88.106		20	4.84
3-Methylpyrazinamine	2-Amino-3-methylpyrazine	C ₅ H ₇ N ₃	19838-08-5	109.130		25	3.39
2-Methylpyrazine		C ₆ H ₈ N ₂	109-08-0	94.115		27	1.45
N-Methyl-4-pyridinamine		C ₆ H ₈ N ₂	1121-58-0	108.141		20	9.65
2-Methylpyridine	2-Picoline	C ₆ H ₇ N	109-06-8	93.127		25	6.00
3-Methylpyridine	3-Picoline	C ₆ H ₇ N	108-99-6	93.127		25	5.70
4-Methylpyridine	4-Picoline	C ₆ H ₇ N	108-89-4	93.127		25	5.99
N-Methylpyrrolidine		C ₅ H ₁₁ N	120-94-5	85.148		25	10.46
2-Methylquinoline	Quinaldine	C ₁₀ H ₉ N	91-63-4	143.185		20	5.83
4-Methylquinoline	Lepidine	C ₁₀ H ₉ N	491-35-0	143.185		20	5.67
5-Methylquinoline		C ₁₀ H ₉ N	7661-55-4	143.185		20	5.20
Methyl Red	Benzoic acid, 2-[[4-(dimethylamino)phenyl]azo]-	C ₁₅ H ₁₅ N ₃ O ₂	493-52-7	269.299	1		2.5
Methyl Red	Benzoic acid, 2-[[4-(dimethylamino)phenyl]azo]-	C ₁₅ H ₁₅ N ₃ O ₂	493-52-7	269.299	2		9.5
Methylsuccinic acid		C ₈ H ₈ O ₄	636-60-2	132.116	1	25	4.13
Methylsuccinic acid		C ₈ H ₈ O ₄	636-60-2	132.116	2	25	5.64
(Methylthio)acetic acid		C ₃ H ₆ O ₂ S	2444-37-3	106.144		25	3.66
2-(Methylthio)aniline		C ₇ H ₉ NS	2987-53-3	139.218		25	3.45
4-(Methylthio)aniline		C ₇ H ₉ NS	104-96-1	139.218		25	4.35
4-(Methylthio)phenol		C ₇ H ₈ OS	1073-72-9	140.203		25	9.53
6-Methyl-1,2,4-triazine-3,5-(2H,4H)-dione	6-Azathymine	C ₄ H ₅ N ₃ O ₂	932-53-6	127.102			7.6
Minoxidil		C ₉ H ₁₅ N ₅ O	38304-91-5	209.248			4.61
Morphine		C ₁₇ H ₁₉ NO ₃	57-27-2	285.338	1	25	8.21
Morphine		C ₁₇ H ₁₉ NO ₃	57-27-2	285.338	2	20	9.85
Morpholine	Tetrahydro-1,4-oxazine	C ₄ H ₉ NO	110-91-8	87.120		25	8.50
Mycophenolic acid		C ₁₇ H ₂₀ O ₆	24280-93-1	320.337			4.5
Nadolol		C ₁₇ H ₂₇ NO ₄	42200-33-9	309.401			9.67
1-Naphthalenecarboxylic acid	1-Naphthoic acid	C ₁₁ H ₈ O ₂	86-55-5	172.181		25	3.69
2-Naphthalenecarboxylic acid	2-Naphthoic acid	C ₁₁ H ₈ O ₂	93-09-4	172.181		25	4.16
1-Naphthol	1-Naphthalenol	C ₁₀ H ₈ O	90-15-3	144.170		25	9.39
2-Naphthol	2-Naphthalenol	C ₁₀ H ₈ O	135-19-3	144.170		25	9.63
1-Naphthylamine	α-Naphthylamine	C ₁₀ H ₉ N	134-32-7	143.185		25	3.92
2-Naphthylamine	β-Naphthylamine	C ₁₀ H ₉ N	91-59-8	143.185		25	4.16
Neobornylamine	1,7,7-Trimethylbicyclo[2.2.1]heptan-2-amine, (1R-exo)-	C ₁₀ H ₁₉ N	2223-67-8	153.265		25	10.01
Neutral Red		C ₁₅ H ₁₇ ClN ₄	553-24-2	288.776			6.7
L-Nicotine	3-(1-Methyl-2-pyrrolidinyl)pyridine, (S)-	C ₁₀ H ₁₄ N ₂	54-11-5	162.231	1		8.02
L-Nicotine	3-(1-Methyl-2-pyrrolidinyl)pyridine, (S)-	C ₁₀ H ₁₄ N ₂	54-11-5	162.231	2		3.12
Nitrotriactic acid	N,N-Bis(carboxymethyl)glycine	C ₆ H ₉ NO ₆	139-13-9	191.138	1	20	3.03
Nitrotriactic acid	N,N-Bis(carboxymethyl)glycine	C ₆ H ₉ NO ₆	139-13-9	191.138	2	20	3.07
Nitrotriactic acid	N,N-Bis(carboxymethyl)glycine	C ₆ H ₉ NO ₆	139-13-9	191.138	3	20	10.70
Nitroacetic acid		C ₂ H ₃ NO ₄	625-75-2	105.050		24	1.48
2-Nitroaniline		C ₆ H ₆ N ₂ O ₂	88-74-4	138.124		25	-0.25
3-Nitroaniline		C ₆ H ₆ N ₂ O ₂	99-09-2	138.124		25	2.46
4-Nitroaniline		C ₆ H ₆ N ₂ O ₂	100-01-6	138.124		25	1.02
Nitrobenzene		C ₆ H ₅ NO ₂	98-95-3	123.110		0	3.98
2-Nitrobenzeneacetic acid	o-Nitrophenylacetic acid	C ₈ H ₇ NO ₄	3740-52-1	181.147		25	4.00
3-Nitrobenzeneacetic acid	m-Nitrophenylacetic acid	C ₈ H ₇ NO ₄	1877-73-2	181.147		25	3.97

4-Nitrobenzoic acid	<i>p</i> -Nitrophenylacetic acid	C ₈ H ₇ NO ₄	104-03-0	181.147		25	3.85
2-Nitrobenzoic acid		C ₇ H ₅ NO ₄	552-16-9	167.120		25	2.17
3-Nitrobenzoic acid		C ₇ H ₅ NO ₄	121-92-6	167.120		25	3.46
4-Nitrobenzoic acid		C ₇ H ₅ NO ₄	62-23-7	167.120		25	3.43
Nitroethane		C ₂ H ₅ NO ₂	79-24-3	75.067		25	8.46
Nitrofurantoin	1-[[[(5-Nitro-2-furyl)methylene]amino]-2,4-imidazolidinedione	C ₈ H ₆ N ₄ O ₅	67-20-9	238.158			7.2
Nitromethane		CH ₃ NO ₂	75-52-5	61.041		25	10.21
2-Nitrophenol		C ₆ H ₅ NO ₃	88-75-5	139.109		25	7.23
3-Nitrophenol		C ₆ H ₅ NO ₃	554-84-7	139.109		25	8.36
4-Nitrophenol		C ₆ H ₅ NO ₃	100-02-7	139.109		25	7.15
3-(2-Nitrophenyl)propanoic acid	2-Nitrobenzenepropanoic acid	C ₉ H ₉ NO ₄	2001-32-3	195.172		25	4.50
3-(4-Nitrophenyl)propanoic acid	4-Nitrobenzenepropanoic acid	C ₉ H ₉ NO ₄	16642-79-8	195.172		25	4.47
4-Nitropyridine		C ₅ H ₄ N ₂ O ₂	1122-61-8	124.098		25	1.61
5-Nitropyrimidinamine		C ₄ H ₄ N ₄ O ₂	3073-77-6	140.101		20	0.35
Nizatidine		C ₁₂ H ₂₁ N ₃ O ₂ S ₂	76963-41-2	331.458	1		2.1
Nizatidine		C ₁₂ H ₂₁ N ₃ O ₂ S ₂	76963-41-2	331.458	2		6.8
Nonanedioic acid	Azelaic acid	C ₉ H ₁₆ O ₄	123-99-9	188.221	1	25	4.53
Nonanedioic acid	Azelaic acid	C ₉ H ₁₆ O ₄	123-99-9	188.221	2	25	5.33
Nonanoic acid	Pelargonic acid	C ₉ H ₁₈ O ₂	112-05-0	158.238		25	4.96
Nonylamine	1-Nonanamine	C ₉ H ₂₁ N	112-20-9	143.270		25	10.64
Norepinephrine	4-(2-Amino-1-hydroxyethyl)-1,2-benzenediol, (1 <i>R</i>)-	C ₈ H ₁₁ NO ₃	51-41-2	169.178	1	25	8.64
Norepinephrine	4-(2-Amino-1-hydroxyethyl)-1,2-benzenediol, (1 <i>R</i>)-	C ₈ H ₁₁ NO ₃	51-41-2	169.178	2	25	9.70
<i>L</i> -Norleucine	2-Aminohexanoic acid, (<i>L</i>)-	C ₆ H ₁₃ NO ₂	327-57-1	131.173	1	25	2.34
<i>L</i> -Norleucine	2-Aminohexanoic acid, (<i>L</i>)-	C ₆ H ₁₃ NO ₂	327-57-1	131.173	2	25	9.83
<i>DL</i> -Norvaline	2-Aminopentanoic acid, (±)-	C ₅ H ₁₁ NO ₂	760-78-1	117.147	1		2.36
<i>DL</i> -Norvaline	2-Aminopentanoic acid, (±)-	C ₅ H ₁₁ NO ₂	760-78-1	117.147	2		9.72
<i>L</i> -Norvaline	2-Aminopentanoic acid, (<i>S</i>)-	C ₅ H ₁₁ NO ₂	6600-40-4	117.147	1	25	2.32
<i>L</i> -Norvaline	2-Aminopentanoic acid, (<i>S</i>)-	C ₅ H ₁₁ NO ₂	6600-40-4	117.147	2	25	9.81
Noscipine		C ₂₂ H ₃₃ NO ₇	128-62-1	413.421			7.8
Novobiocin	Streptonivcin	C ₃₁ H ₃₆ N ₂ O ₁₁	303-81-1	612.624	1		4.3
Novobiocin	Streptonivcin	C ₃₁ H ₃₆ N ₂ O ₁₁	303-81-1	612.624	2		9.1
<i>cis,cis</i> -9,12-Octadecadienoic acid	Linoleic acid	C ₁₈ H ₃₂ O ₂	60-33-3	280.446			7.6
Octadecylamine	1-Octadecanamine	C ₁₈ H ₃₉ N	124-30-1	269.510		25	10.60
1,8-Octanediamine		C ₈ H ₂₀ N ₂	373-44-4	144.258	1	20	11.00
1,8-Octanediamine		C ₈ H ₂₀ N ₂	373-44-4	144.258	2	20	10.1
Octanedioic acid	Suberic acid	C ₈ H ₁₄ O ₄	505-48-6	174.195	1	25	4.52
Octanoic acid	Caprylic acid	C ₈ H ₁₆ O ₂	124-07-2	144.212		25	4.89
Octylamine	1-Octanamine	C ₈ H ₁₉ N	111-86-4	129.244		25	10.65
Oleanolic acid		C ₃₀ H ₄₈ O ₃	508-02-1	456.700			2.52
<i>L</i> -Ornithine	2,5-Diaminopentanoic acid, (<i>S</i>)-	C ₅ H ₁₂ N ₂ O ₂	70-26-8	132.161	1	25	1.71
<i>L</i> -Ornithine	2,5-Diaminopentanoic acid, (<i>S</i>)-	C ₅ H ₁₂ N ₂ O ₂	70-26-8	132.161	2	25	8.69
<i>L</i> -Ornithine	2,5-Diaminopentanoic acid, (<i>S</i>)-	C ₅ H ₁₂ N ₂ O ₂	70-26-8	132.161	3	25	10.76
Oxalic acid		C ₂ H ₂ O ₄	144-62-7	90.035	1	25	1.25
Oxalic acid		C ₂ H ₂ O ₄	144-62-7	90.035	2	25	3.81
Oxaloacetic acid	Oxalacetic acid	C ₄ H ₄ O ₅	328-42-7	132.072	1	25	2.55
Oxaloacetic acid	Oxalacetic acid	C ₄ H ₄ O ₅	328-42-7	132.072	2	25	4.37
Oxaloacetic acid	Oxalacetic acid	C ₄ H ₄ O ₅	328-42-7	132.072	3	25	13.03
Oxazole		C ₃ H ₃ NO	288-42-6	69.062		33	0.8
2-Oxobutanoic acid		C ₄ H ₆ O ₃	600-18-0	102.089		25	2.50
2-Oxoglutaric acid	α-Ketoglutaric acid	C ₅ H ₆ O ₅	328-50-7	146.099	1	25	2.47
2-Oxoglutaric acid	α-Ketoglutaric acid	C ₅ H ₆ O ₅	328-50-7	146.099	2	25	4.68
Papaverine		C ₂₀ H ₂₁ NO ₄	58-74-2	339.386			6.4
Pentadecylamine	Pentadecanamine	C ₁₅ H ₃₃ N	2570-26-5	227.430		25	10.61
Pentafluorobenzoic acid		C ₇ HF ₅ O ₂	602-94-8	212.074		25	1.75
1,2,2,6,6-Pentamethylpiperidine	Pempidine	C ₁₀ H ₂₁ N	79-55-0	155.281		30	11.25
3-Pentanamine		C ₅ H ₁₃ N	616-24-0	87.164		17	10.59
1,5-Pentanediamine	Cadaverine	C ₅ H ₁₄ N ₂	462-94-2	102.178	1	25	10.05

1,5-Pentanediamine	Cadaverine	C ₅ H ₁₄ N ₂	462-94-2	102.178	2	25	10.93
Pentanedioic acid	Glutaric acid	C ₅ H ₈ O ₄	110-94-1	132.116	1	18	4.32
Pentanedioic acid	Glutaric acid	C ₅ H ₈ O ₄	110-94-1	132.116	2	25	5.42
Pentanoic acid	Valeric acid	C ₅ H ₁₀ O ₂	109-52-4	102.132		20	4.83
<i>trans</i> -3-Pentenoic acid		C ₅ H ₈ O ₂	1617-32-9	100.117		25	4.51
Pentostatin		C ₁₁ H ₁₆ N ₄ O ₄	53910-25-1	268.270			5.2
Pentylamine	Amylamine	C ₅ H ₁₃ N	110-58-7	87.164		25	10.63
Perfludone	4-(Phenylsulfonyl)- <i>N</i> -[(trifluoromethyl)sulfonyl]- <i>o</i> -toluidine	C ₁₄ H ₁₂ F ₃ NO ₄ S ₂	37924-13-3	379.375			2.5
1 <i>H</i> -Perimidine		C ₁₁ H ₈ N ₂	204-02-4	168.195		20	6.35
Phenanthridine		C ₁₃ H ₉ N	229-87-8	179.217		20	5.58
1,10-Phenanthroline	<i>o</i> -Phenanthroline	C ₁₂ H ₈ N ₂	66-71-7	180.205		25	4.84
Phenazine	Dibenzopyrazine	C ₁₂ H ₈ N ₂	92-82-0	180.205		20	1.20
Phenobarbital	5-Ethyl-5-phenyl-2,4,6(1 <i>H</i> ,3 <i>H</i> ,5 <i>H</i>)-pyrimidinetrione	C ₁₂ H ₁₂ N ₂ O ₃	50-06-6	232.234	1		7.3
Phenobarbital	5-Ethyl-5-phenyl-2,4,6(1 <i>H</i> ,3 <i>H</i> ,5 <i>H</i>)-pyrimidinetrione	C ₁₂ H ₁₂ N ₂ O ₃	50-06-6	232.234	2		11.8
Phenol	Hydroxybenzene	C ₆ H ₆ O	108-95-2	94.111		25	9.99
Phenolphthalein	3,3-Bis(4-hydroxyphenyl)-1(3 <i>H</i>)-isobenzofuranone	C ₂₀ H ₁₄ O ₄	77-09-8	318.323		25	9.7
Phenol Red	Phenolsulfonphthalein	C ₁₀ H ₁₄ O ₆ S	143-74-8	354.376			7.9
Phenoxyacetic acid		C ₈ H ₈ O ₃	122-59-8	152.148		25	3.17
2-Phenoxybenzoic acid		C ₁₃ H ₁₀ O ₃	2243-42-7	214.216		25	3.53
3-Phenoxybenzoic acid		C ₁₃ H ₁₀ O ₃	3739-38-6	214.216		25	3.95
4-Phenoxybenzoic acid		C ₁₃ H ₁₀ O ₃	2215-77-2	214.216		25	4.57
2-(3-Phenoxyphenyl)propanoic acid, (±)-	Fenoprofen	C ₁₅ H ₁₄ O ₃	31879-05-7	242.270			7.3
<i>L</i> -Phenylalanine	α-Aminobenzenepropanoic acid, (S)-	C ₉ H ₁₁ NO ₂	63-91-2	165.189	1	25	2.20
<i>L</i> -Phenylalanine	α-Aminobenzenepropanoic acid, (S)-	C ₉ H ₁₁ NO ₂	63-91-2	165.189	2	25	9.31
α-Phenylbenzeneacetic acid	Diphenylacetic acid	C ₁₄ H ₁₂ O ₂	117-34-0	212.244		25	3.94
2-Phenylbenzimidazole	Phenizidole	C ₁₃ H ₁₀ N ₂	716-79-0	194.231	1	25	5.23
2-Phenylbenzimidazole	Phenizidole	C ₁₃ H ₁₀ N ₂	716-79-0	194.231	2	25	11.91
2-Phenylbenzoic acid		C ₁₃ H ₁₀ O ₂	947-84-2	198.217		25	3.46
Phenyl biguanide	<i>N</i> -Phenylimidodicarbonimidic diamide	C ₈ H ₁₁ N ₅	102-02-3	177.207	1		10.76
Phenyl biguanide	<i>N</i> -Phenylimidodicarbonimidic diamide	C ₈ H ₁₁ N ₅	102-02-3	177.207	2		2.13
Phenylbutazone		C ₁₉ H ₂₀ N ₂ O ₂	50-33-9	308.374			4.5
<i>N</i> -Phenylglycine	Phenylaminoacetic acid	C ₈ H ₉ NO ₂	103-01-5	151.163	1	25	1.83
<i>N</i> -Phenylglycine	Phenylaminoacetic acid	C ₈ H ₉ NO ₂	103-01-5	151.163	2		4.39
Phenylhydrazine		C ₆ H ₈ N ₂	100-63-0	108.141		15	8.79
Phenylpropanolamine hydrochloride	α-(1-Aminoethyl)benzenemethanol hydrochloride, (R*,S*)-(±)-	C ₉ H ₁₁ ClNO	154-41-6	187.666			9.44
Phthalazine	2,3-Benzodiazine	C ₈ H ₆ N ₂	253-52-1	130.147		20	3.47
Phthalic acid	1,2-Benzenedicarboxylic acid	C ₈ H ₆ O ₄	88-99-3	166.132	1	25	2.943
Phthalic acid	1,2-Benzenedicarboxylic acid	C ₈ H ₆ O ₄	88-99-3	166.132	2	25	5.432
Physostigmine		C ₁₅ H ₂₁ N ₃ O ₂	57-47-6	275.347	1		6.12
Physostigmine		C ₁₅ H ₂₁ N ₃ O ₂	57-47-6	275.347	2		12.24
Pilocarpine		C ₁₁ H ₁₆ N ₂ O ₂	92-13-7	208.257	1	25	1.6
Pilocarpine		C ₁₁ H ₁₆ N ₂ O ₂	92-13-7	208.257	2	25	6.9
Piperazine	Diethylenediamine	C ₄ H ₁₀ N ₂	110-85-0	86.135	1	25	9.73
Piperazine	Diethylenediamine	C ₄ H ₁₀ N ₂	110-85-0	86.135	2	25	5.33
Piperidine	Azacyclohexane	C ₅ H ₁₁ N	110-89-4	85.148		25	11.123
2-Piperidinecarboxylic acid	Pipecolic acid	C ₆ H ₁₁ NO ₂	535-75-1	129.157	1	25	2.28
2-Piperidinecarboxylic acid	Pipecolic acid	C ₆ H ₁₁ NO ₂	535-75-1	129.157	2	25	10.72
Piperine		C ₁₇ H ₁₉ NO ₃	94-62-2	285.338		18	12.22
<i>L</i> -Proline	2-Pyrrolidinecarboxylic acid	C ₅ H ₉ NO ₂	147-85-3	115.131	1	25	1.95
<i>L</i> -Proline	2-Pyrrolidinecarboxylic acid	C ₅ H ₉ NO ₂	147-85-3	115.131	2	25	10.64
1,2-Propanediamine, (±)-	Propylenediamine	C ₃ H ₁₀ N ₂	10424-38-1	74.124	1	25	9.82
1,2-Propanediamine, (±)-	Propylenediamine	C ₃ H ₁₀ N ₂	10424-38-1	74.124	2	25	6.61
1,3-Propanediamine	1,3-Diaminopropane	C ₃ H ₁₀ N ₂	109-76-2	74.124	1	25	10.55
1,3-Propanediamine	1,3-Diaminopropane	C ₃ H ₁₀ N ₂	109-76-2	74.124	2	25	8.88
1,2,3-Propanetriamine	1,2,3-Triaminopropane	C ₃ H ₁₁ N ₃	21291-99-6	89.139	1	20	9.59
1,2,3-Propanetriamine	1,2,3-Triaminopropane	C ₃ H ₁₁ N ₃	21291-99-6	89.139	2	20	7.95
Propanoic acid	Propionic acid	C ₃ H ₆ O ₂	79-09-4	74.079		25	4.87

2-Propanone oxime	Acetoxime	C ₃ H ₇ NO	127-06-0	73.094		25	12.42
Propargyl alcohol	3-Hydroxy-1-propyne	C ₃ H ₄ O	107-19-7	56.063		25	13.6
<i>trans</i> -1-Propene-1,2-dicarboxylic acid	Mesaconic acid	C ₅ H ₆ O ₄	498-24-8	130.100	1	25	3.09
<i>trans</i> -1-Propene-1,2,3-tricarboxylic acid	Mesaconic acid	C ₅ H ₆ O ₄	498-24-8	130.100	2	25	4.75
1-Propene-2,3-dicarboxylic acid	Itaconic acid	C ₅ H ₆ O ₄	97-65-4	130.100	1	25	3.85
1-Propene-2,3-dicarboxylic acid	Itaconic acid	C ₅ H ₆ O ₄	97-65-4	130.100	2	25	5.45
<i>cis</i> -1-Propene-1,2,3-tricarboxylic acid	<i>cis</i> -Aconitic acid	C ₆ H ₆ O ₆	585-84-2	174.108		25	1.95
<i>trans</i> -1-Propene-1,2,3-tricarboxylic acid	<i>trans</i> -Aconitic acid	C ₆ H ₆ O ₆	4023-65-8	174.108	1	25	2.80
<i>trans</i> -1-Propene-1,2,3-tricarboxylic acid	<i>trans</i> -Aconitic acid	C ₆ H ₆ O ₆	4023-65-8	174.108	2	25	4.46
Propylamine	1-Propanamine	C ₃ H ₇ N	107-10-8	59.110		25	10.54
<i>N</i> -Propylglycine		C ₅ H ₁₁ NO ₂	25303-14-4	117.147	1	25	2.35
<i>N</i> -Propylglycine		C ₅ H ₁₁ NO ₂	25303-14-4	117.147	2	25	10.19
2-Propylpentanoic acid	Valproic acid	C ₈ H ₁₆ O ₂	99-66-1	144.212			4.6
2-Propylpiperidine, (S)-	Coniine	C ₈ H ₁₇ N	458-88-8	127.228			10.9
<i>trans</i> -6-Propyl-3-piperidinol, (3S)-	Pseudoconhydrine	C ₈ H ₁₇ NO	140-55-6	143.227			10.3
Propyl 3,4,5-trihydroxybenzoate	Propyl gallate	C ₁₀ H ₁₂ O ₅	121-79-9	212.199			8.11
2-Propynoic acid	Propiolic acid	C ₃ H ₂ O ₂	471-25-0	70.047		25	1.84
Protriptyline		C ₁₉ H ₂₁ N	438-60-8	263.377			8.2
Pseudotropine	8-Methyl-8-azabicyclo[3.2.1]octan-3-ol, <i>exo</i>	C ₈ H ₁₅ NO	135-97-7	141.211		15	3.80
Pteridine	Pyrazino[2,3- <i>d</i>]pyrimidine	C ₆ H ₄ N ₄	91-18-9	132.123		20	4.05
1 <i>H</i> -Purine	6 <i>H</i> -Imidazo[4,5- <i>d</i>]pyrimidine	C ₅ H ₄ N ₄	120-73-0	120.113	1	20	2.30
1 <i>H</i> -Purine	6 <i>H</i> -Imidazo[4,5- <i>d</i>]pyrimidine	C ₅ H ₄ N ₄	120-73-0	120.113	2	20	8.96
Pyrazine	1,4-Diazine	C ₄ H ₄ N ₂	290-37-9	80.088		20	0.65
Pyrazinecarboxamide	Pyrazinamide	C ₅ H ₅ N ₃ O	98-96-4	123.113			0.5
1 <i>H</i> -Pyrazole	1,2-Diazole	C ₃ H ₄ N ₂	288-13-1	68.077		25	2.49
Pyridazine	1,2-Diazabenzene	C ₄ H ₄ N ₂	289-80-5	80.088		20	2.24
2-Pyridinamine	2-Aminopyridine	C ₅ H ₆ N ₂	504-29-0	94.115		20	6.82
3-Pyridinamine	3-Aminopyridine	C ₅ H ₆ N ₂	462-08-8	94.115		25	6.04
4-Pyridinamine	4-Aminopyridine	C ₅ H ₆ N ₂	504-24-5	94.115		25	9.11
Pyridine	Azine	C ₅ H ₅ N	110-86-1	79.101		25	5.23
2-Pyridinecarboxaldehyde		C ₆ H ₅ NO	1121-60-4	107.110		25	12.68
4-Pyridinecarboxaldehyde		C ₆ H ₅ NO	872-85-5	107.110		30	12.05
2-Pyridinecarboxaldehyde oxime		C ₆ H ₆ N ₂ O	873-69-8	122.124	1	20	3.59
2-Pyridinecarboxaldehyde oxime		C ₆ H ₆ N ₂ O	873-69-8	122.124	2	20	10.18
3-Pyridinecarboxamide	Niacinamide	C ₆ H ₆ N ₂ O	98-92-0	122.124		20	3.3
2-Pyridinecarboxylic acid	Picolinic acid	C ₆ H ₅ NO ₂	98-98-6	123.110	1	20	0.99
2-Pyridinecarboxylic acid	Picolinic acid	C ₆ H ₅ NO ₂	98-98-6	123.110	2	20	5.39
3-Pyridinecarboxylic acid	Nicotinic acid	C ₆ H ₅ NO ₂	59-67-6	123.110	1	25	2.00
3-Pyridinecarboxylic acid	Nicotinic acid	C ₆ H ₅ NO ₂	59-67-6	123.110	2	25	4.82
4-Pyridinecarboxylic acid	Isonicotinic acid	C ₆ H ₅ NO ₂	55-22-1	123.110	1	25	1.77
4-Pyridinecarboxylic acid	Isonicotinic acid	C ₆ H ₅ NO ₂	55-22-1	123.110	2	25	4.84
2,5-Pyridinediamine	2,5-Diaminopyridine	C ₅ H ₇ N ₃	4318-76-7	109.130		20	6.48
2,3-Pyridinedicarboxylic acid	Quinolinic acid	C ₇ H ₅ NO ₄	89-00-9	167.120	1	25	2.43
2,3-Pyridinedicarboxylic acid	Quinolinic acid	C ₇ H ₅ NO ₄	89-00-9	167.120	2	25	4.78
2,4-Pyridinedicarboxylic acid	Lutidinic acid	C ₇ H ₅ NO ₄	499-80-9	167.120	1	25	2.15
2,6-Pyridinedicarboxylic acid	Dipicolinic acid	C ₇ H ₅ NO ₄	499-83-2	167.120	1	25	2.16
2,6-Pyridinedicarboxylic acid	Dipicolinic acid	C ₇ H ₅ NO ₄	499-83-2	167.120	2	25	4.76
3,5-Pyridinedicarboxylic acid	Dinicotinic acid	C ₇ H ₅ NO ₄	499-81-0	167.120	1	25	2.80
Pyridine-1-oxide	Pyridine <i>N</i> -oxide	C ₅ H ₅ NO	694-59-7	95.100		24	0.79
2-Pyridinol		C ₅ H ₅ NO	72762-00-6	95.100	1	20	0.75
2-Pyridinol		C ₅ H ₅ NO	72762-00-6	95.100	2	20	11.65
3-Pyridinol		C ₅ H ₅ NO	109-00-2	95.100	1	20	4.79
3-Pyridinol		C ₅ H ₅ NO	109-00-2	95.100	2	20	8.75
4-Pyridinol		C ₅ H ₅ NO	626-64-2	95.100	1	20	3.20
4-Pyridinol		C ₅ H ₅ NO	626-64-2	95.100	2	20	11.12
2(1 <i>H</i>)-Pyridinone		C ₅ H ₅ NO	142-08-5	95.100	1	20	0.75
2(1 <i>H</i>)-Pyridinone		C ₅ H ₅ NO	142-08-5	95.100	2	20	11.65
2-Pyrimidinamine		C ₄ H ₅ N ₃	109-12-6	95.103		20	3.45
4-Pyrimidinamine		C ₄ H ₅ N ₃	591-54-8	95.103		20	5.71

Pyrimidine	1,3-Diazine	C ₄ H ₄ N ₂	289-95-2	80.088		20	1.23
2,4,6-Pyrimidinetriamine		C ₄ H ₇ N ₅	1004-38-2	125.133		20	6.84
Pyrocatechol	1,2-Benzenediol	C ₆ H ₆ O ₂	120-80-9	110.111	1	25	9.34
Pyrocatechol	1,2-Benzenediol	C ₆ H ₆ O ₂	120-80-9	110.111	2	25	12.6
L-Pyrogutamic acid	5-Oxo-L-proline	C ₅ H ₇ NO ₃	98-79-3	129.115		25	3.32
Pyrrrole	Imidole	C ₄ H ₅ N	109-97-7	67.090		25	-3.8
1H-Pyrrrole-2-carboxylic acid		C ₅ H ₅ NO ₂	634-97-9	111.100		20	4.45
1H-Pyrrrole-3-carboxylic acid	3-Pyrrrolicarboxylic acid	C ₅ H ₅ NO ₂	931-03-3	111.100		20	5.00
Pyrrrolidine	Azacyclopentane	C ₄ H ₈ N	123-75-1	71.121		25	11.31
Pyruvic acid		C ₃ H ₄ O ₃	127-17-3	88.062		25	2.39
Quinazoline	1,3-Benzodiazine	C ₈ H ₆ N ₂	253-82-7	130.147		29	3.43
Quinidine		C ₂₀ H ₂₄ N ₂ O ₂	56-54-2	324.417	1	20	5.4
Quinidine		C ₂₀ H ₂₄ N ₂ O ₂	56-54-2	324.417	2	20	10.0
Quinine	6'-Methoxycinchonan-9-ol, (8 α ,9R)-	C ₂₀ H ₂₄ N ₂ O ₂	130-95-0	324.417	1	25	8.52
Quinine	6'-Methoxycinchonan-9-ol, (8 α ,9R)-	C ₂₀ H ₂₄ N ₂ O ₂	130-95-0	324.417	2	25	4.13
2-Quinolinamine	2-Aminoquinoline	C ₉ H ₈ N ₂	580-22-3	144.173		20	7.34
3-Quinolinamine	3-Aminoquinoline	C ₉ H ₈ N ₂	580-17-6	144.173		20	4.91
4-Quinolinamine	4-Aminoquinoline	C ₉ H ₈ N ₂	578-68-7	144.173		20	9.17
Quinoline	1-Azanaphthalene	C ₉ H ₇ N	91-22-5	129.159		20	4.90
8-Quinolincarboxylic acid	8-Carboxyquinoline	C ₁₀ H ₇ NO ₂	86-59-9	173.169		25	1.82
2-Quinolinol	2-Hydroxyquinoline	C ₉ H ₇ NO	59-31-4	145.158	1	20	-0.31
2-Quinolinol	2-Hydroxyquinoline	C ₉ H ₇ NO	59-31-4	145.158	2	20	11.76
3-Quinolinol	3-Hydroxyquinoline	C ₉ H ₇ NO	580-18-7	145.158	1	20	4.28
3-Quinolinol	3-Hydroxyquinoline	C ₉ H ₇ NO	580-18-7	145.158	2	20	8.08
4-Quinolinol	4-Hydroxyquinoline	C ₉ H ₇ NO	611-36-9	145.158	1	20	2.23
4-Quinolinol	4-Hydroxyquinoline	C ₉ H ₇ NO	611-36-9	145.158	2	20	11.28
6-Quinolinol	6-Hydroxyquinoline	C ₉ H ₇ NO	580-16-5	145.158	1	20	5.15
6-Quinolinol	6-Hydroxyquinoline	C ₉ H ₇ NO	580-16-5	145.158	2	20	8.90
8-Quinolinol	8-Hydroxyquinoline	C ₉ H ₇ NO	148-24-3	145.158	1	25	4.91
8-Quinolinol	8-Hydroxyquinoline	C ₉ H ₇ NO	148-24-3	145.158	2	25	9.81
Quinoxaline	1,4-Benzodiazine	C ₈ H ₆ N ₂	91-19-0	130.147		20	0.56
Reserpine		C ₂₃ H ₄₀ N ₂ O ₉	50-55-5	608.679			6.6
Resorcinol	1,3-Benzenediol	C ₆ H ₆ O ₂	108-46-3	110.111	1	25	9.32
Resorcinol	1,3-Benzenediol	C ₆ H ₆ O ₂	108-46-3	110.111	2	25	11.1
Riboflavin		C ₁₇ H ₂₀ N ₄ O ₆	83-88-5	376.364	1		1.7
Riboflavin		C ₁₇ H ₂₀ N ₄ O ₆	83-88-5	376.364	2	25	9.69
L-Ribose		C ₅ H ₁₀ O ₅	24259-59-4	150.130		25	12.22
Rifampin		C ₄₃ H ₅₈ N ₄ O ₁₂	13292-46-1	822.941	1		1.7
Rifampin		C ₄₃ H ₅₈ N ₄ O ₁₂	13292-46-1	822.941	2		7.9
Saccharin		C ₇ H ₅ NO ₂ S	81-07-2	183.185		18	11.68
Salicylaldehyde	2-Hydroxybenzaldehyde	C ₇ H ₆ O ₂	90-02-8	122.122		25	8.37
Sarcosine	N-Methylglycine	C ₃ H ₇ NO ₂	107-97-1	89.094	1	25	2.21
Sarcosine	N-Methylglycine	C ₃ H ₇ NO ₂	107-97-1	89.094	2	25	10.1
Sebacic acid		C ₁₀ H ₁₈ O ₄	111-20-6	202.248	1		4.59
Sebacic acid		C ₁₀ H ₁₈ O ₄	111-20-6	202.248	2		5.59
L-Serine	2-Amino-3-hydroxypropanoic acid, (S)-	C ₃ H ₇ NO ₃	56-45-1	105.093	1	25	2.19
L-Serine	2-Amino-3-hydroxypropanoic acid, (S)-	C ₃ H ₇ NO ₃	56-45-1	105.093	2	25	9.21
Solanine		C ₄₅ H ₇₃ NO ₁₅	20562-02-1	868.060		15	6.66
Sparteine		C ₁₅ H ₂₆ N ₂	90-39-1	234.380	1	20	2.24
Sparteine		C ₁₅ H ₂₆ N ₂	90-39-1	234.380	2	20	9.46
Strychnine		C ₂₁ H ₂₂ N ₂ O ₂	57-24-9	334.412		25	8.26
Succinic acid	Butanedioic acid	C ₄ H ₆ O ₄	110-15-6	118.089	1	25	4.21
Succinic acid	Butanedioic acid	C ₄ H ₆ O ₄	110-15-6	118.089	2	25	5.64
Succinimide		C ₄ H ₅ NO ₂	123-56-8	99.089		25	9.62
Sucrose		C ₁₂ H ₂₂ O ₁₁	57-50-1	342.296		25	12.7
Sulfabenzamide	N-[(4-Aminophenyl)sulfonyl]benzamide	C ₁₃ H ₁₂ N ₂ O ₂ S	127-71-9	276.310		25	4.57
Sulfacytine		C ₁₂ H ₁₄ N ₄ O ₂ S	17784-12-2	294.329			6.9
Sulfamethazine		C ₁₂ H ₁₄ N ₄ O ₂ S	57-68-1	278.330	1		7.4
Sulfamethazine		C ₁₂ H ₁₄ N ₄ O ₂ S	57-68-1	278.330	2		2.65

Sulfamethoxypyridazine		C ₁₁ H ₁₂ N ₄ O ₂ S	80-35-3	280.303			6.7
Sulfathiazole	4-Amino- <i>N</i> -2-thiazolylbenzenesulfonamide	C ₉ H ₈ N ₂ O ₂ S ₂	72-14-0	255.316			7.2
Sulfisoxazole		C ₁₁ H ₁₃ N ₃ O ₂ S	127-69-5	267.304			5
<i>DL</i> -Tartaric acid	2,3-Dihydroxybutanedioic acid, (<i>R</i> *, <i>R</i> *)-(±)-	C ₄ H ₆ O ₆	133-37-9	150.087	1	25	3.03
<i>DL</i> -Tartaric acid	2,3-Dihydroxybutanedioic acid, (<i>R</i> *, <i>R</i> *)-(±)-	C ₄ H ₆ O ₆	133-37-9	150.087	2	25	4.37
<i>meso</i> -Tartaric acid	2,3-Dihydroxybutanedioic acid, (<i>R</i> *, <i>R</i> *)-	C ₄ H ₆ O ₆	147-73-9	150.087	1	25	3.17
<i>meso</i> -Tartaric acid	2,3-Dihydroxybutanedioic acid, (<i>R</i> *, <i>R</i> *)-	C ₄ H ₆ O ₆	147-73-9	150.087	2	25	4.91
<i>L</i> -Tartaric acid	2,3-Dihydroxybutanedioic acid, [<i>R</i> -(<i>R</i> *, <i>R</i> *)]-	C ₄ H ₆ O ₆	87-69-4	150.087	1	25	2.98
<i>L</i> -Tartaric acid	2,3-Dihydroxybutanedioic acid, [<i>R</i> -(<i>R</i> *, <i>R</i> *)]-	C ₄ H ₆ O ₆	87-69-4	150.087	2	25	4.34
Taurocholic acid	Cholaic acid	C ₂₆ H ₄₅ NO ₇ S	81-24-3	515.703			1.4
Teniposide		C ₃₂ H ₃₂ O ₁₃ S	29767-20-2	656.653			10.13
Terephthalic acid	1,4-Benzenedicarboxylic acid	C ₈ H ₆ O ₄	100-21-0	166.132	1	25	3.54
Terephthalic acid	1,4-Benzenedicarboxylic acid	C ₈ H ₆ O ₄	100-21-0	166.132	2	25	4.34
Tetradecylamine	1-Tetradecanamine	C ₁₄ H ₃₁ N	2016-42-4	213.403		25	10.62
5,6,7,8-Tetrahydro-2-naphthol	5,6,7,8-Tetrahydro-β-naphthol	C ₁₀ H ₁₂ O	1125-78-6	148.201		25	10.48
<i>N,N,N',N'</i> -Tetramethyl-1,2-ethanediamine	1,2-Dimethylaminoethane	C ₆ H ₁₆ N ₂	110-18-9	116.204	1	25	10.40
<i>N,N,N',N'</i> -Tetramethyl-1,2-ethanediamine	1,2-Dimethylaminoethane	C ₆ H ₁₆ N ₂	110-18-9	116.204	2	25	8.26
2,2,6,6-Tetramethylpiperidine	Norpempidine	C ₉ H ₁₉ N	768-66-1	141.254		25	11.07
Tetramethylurea		C ₅ H ₁₂ N ₂ O	632-22-4	116.161			2
Tetradotoxin		C ₁₁ H ₁₇ N ₃ O ₈	4368-28-9	319.268			8.76
Thebaine		C ₁₉ H ₂₁ NO ₃	115-37-7	311.375		15	6.05
Theobromine		C ₇ H ₈ N ₄ O ₂	83-67-0	180.165		18	7.89
Theophylline	3,7-Dihydro-1,3-dimethyl-1 <i>H</i> -purine-2,6-dione	C ₇ H ₈ N ₄ O ₂	58-55-9	180.165	1	25	8.77
2-Thiazolamine	2-Aminothiazole	C ₃ H ₄ N ₂ S	96-50-4	100.142		20	5.36
Thiazole		C ₃ H ₃ NS	288-47-1	85.128		25	2.52
Thioacetic acid		C ₂ H ₄ OS	507-09-5	76.117		25	3.33
Thioctic acid	1,2-Dithiolane-3-pentanoic acid	C ₈ H ₁₄ O ₂ S ₂	62-46-4	206.326			5.4
Thioglycolic acid		C ₂ H ₄ O ₂ S	68-11-1	92.117		25	3.68
2-Thiophenecarboxylic acid	2-Carboxythiophene	C ₅ H ₄ O ₂ S	527-72-0	128.150		25	3.49
3-Thiophenecarboxylic acid	3-Thenoic acid	C ₅ H ₄ O ₂ S	88-13-1	128.150		25	4.1
Thiourea	Thiocarbamide	CH ₄ N ₂ S	62-56-6	76.121		25	-1
<i>L</i> -Threonine	2-Amino-3-hydroxybutanoic acid, [<i>R</i> -(<i>R</i> *, <i>S</i> *)]	C ₄ H ₉ NO ₃	72-19-5	119.119	1	25	2.09
<i>L</i> -Threonine	2-Amino-3-hydroxybutanoic acid, [<i>R</i> -(<i>R</i> *, <i>S</i> *)]	C ₄ H ₉ NO ₃	72-19-5	119.119	2	25	9.10
Thymine		C ₅ H ₈ N ₂ O ₂	65-71-4	126.114		25	9.94
<i>L</i> -Thyroxine		C ₁₅ H ₁₁ I ₄ NO ₄	51-48-9	776.871	1	25	2.2
<i>L</i> -Thyroxine		C ₁₅ H ₁₁ I ₄ NO ₄	51-48-9	776.871	2	25	6.45
<i>L</i> -Thyroxine		C ₁₅ H ₁₁ I ₄ NO ₄	51-48-9	776.871	3	25	10.1
Tolazamide		C ₁₄ H ₂₁ N ₃ O ₂ S	1156-19-0	311.400		25	3.6
<i>o</i> -Toluic acid		C ₈ H ₈ O ₂	118-90-1	136.149		25	3.91
<i>m</i> -Toluic acid		C ₈ H ₈ O ₂	99-04-7	136.149		25	4.25
<i>p</i> -Toluic acid		C ₈ H ₈ O ₂	99-94-5	136.149		25	4.37
1,3,5-Triazine-2,4,6-triamine	Melamine	C ₃ H ₆ N ₆	108-78-1	126.120		25	5.00
1 <i>H</i> -1,2,3-Triazole		C ₂ H ₃ N ₃	288-36-8	69.065		20	1.17
1 <i>H</i> -1,2,4-Triazole	Pyrotriazole	C ₂ H ₃ N ₃	288-88-0	69.065		20	2.27
Trichloroacetaldehyde	Chloral	C ₂ HCl ₃ O	75-87-6	147.387		25	10.04
Trichloroacetic acid		C ₂ HCl ₃ O ₂	76-03-9	163.387		20	0.66
2,2,2-Trichloroethanol		C ₂ H ₃ Cl ₃ O	115-20-8	149.403		25	12.24
Triclopyr	Acetic acid, [(3,5,6-trichloro-2-pyridinyl)oxy]-	C ₇ H ₄ Cl ₃ NO ₃	55335-06-3	256.471			2.68
(Tridecyl)amine	1-Tridecanamine	C ₁₃ H ₂₉ N	2869-34-3	199.376		25	10.63
Triethanolamine	Tris(2-hydroxyethyl)amine	C ₆ H ₁₅ NO ₃	102-71-6	149.188		25	7.76
Triethylamine	<i>N,N</i> -Diethylethanamine	C ₆ H ₁₃ N	121-44-8	101.190		25	10.75
Triethylenediamine		C ₆ H ₁₂ N ₂	280-57-9	112.172	1		3.0
Triethylenediamine		C ₆ H ₁₂ N ₂	280-57-9	112.172	2		8.7
Trifluoroacetic acid		C ₂ HF ₃ O ₂	76-05-1	114.023		25	0.52
2,2,2-Trifluoroethanol		C ₂ H ₃ F ₃ O	75-89-8	100.039		25	12.37
3-(Trifluoromethyl)aniline		C ₇ H ₆ F ₃ N	98-16-8	161.125		25	3.49
4-(Trifluoromethyl)aniline		C ₇ H ₆ F ₃ N	455-14-1	161.125		25	2.45
2-(Trifluoromethyl)phenol		C ₇ H ₅ F ₃ O	444-30-4	162.109		25	8.95
3-(Trifluoromethyl)phenol		C ₇ H ₅ F ₃ O	98-17-9	162.109		25	8.68

2,4,6-Trihydroxybenzoic acid		C ₇ H ₆ O ₅	83-30-7	170.120		25	1.68
3,4,5-Trihydroxybenzoic acid	Gallic acid	C ₇ H ₆ O ₅	149-91-7	170.120		25	4.41
Trimethoprim		C ₁₄ H ₁₈ N ₄ O ₃	738-70-5	290.318			6.6
Trimethylamine	<i>N,N</i> -Dimethylmethanamine	C ₃ H ₉ N	75-50-3	59.110		25	9.80
Trimethylamine oxide	<i>N,N</i> -Dimethylmethanamine oxide	C ₃ H ₉ NO	1184-78-7	75.109		20	4.65
2,2,4-Trimethylpiperidine		C ₈ H ₁₇ N	101257-71-0	127.228		30	11.04
2,4,6-Trimethylpyridine	2,4,6-Collidine	C ₈ H ₁₁ N	108-75-8	121.180		25	7.43
2,4,6-Trinitrobenzoic acid		C ₇ H ₃ N ₃ O ₈	129-66-8	257.114		25	0.65
2,4,6-Trinitrophenol	Picric acid	C ₆ H ₃ N ₃ O ₇	88-89-1	229.104		24	0.42
Tris(hydroxymethyl)methylamine	2-Amino-2-(hydroxymethyl)-1,3-propanediol	C ₄ H ₁₁ NO ₃	77-86-1	121.135		20	8.3
Tropacocaine		C ₁₅ H ₁₉ N ₂ O ₂	537-26-8	245.318		15	4.32
Tropine	8-Methyl-8-azabicyclo[3.2.1]octan-3-ol, <i>endo</i>	C ₈ H ₁₅ NO	120-29-6	141.211		15	3.80
Tryptamine		C ₁₀ H ₁₂ N ₂	61-54-1	160.215		25	10.2
<i>L</i> -Tryptophan	α -Aminoindole-3-propanoic acid, (<i>l</i> -)	C ₁₁ H ₁₂ N ₂ O ₂	73-22-3	204.225	1	25	2.46
<i>L</i> -Tryptophan	α -Aminoindole-3-propanoic acid, (<i>l</i> -)	C ₁₁ H ₁₂ N ₂ O ₂	73-22-3	204.225	2	25	9.41
<i>L</i> -Tyrosine	4-Hydroxy- <i>L</i> -phenylalanine	C ₉ H ₁₁ NO ₃	60-18-4	181.188	1	25	2.20
<i>L</i> -Tyrosine	4-Hydroxy- <i>L</i> -phenylalanine	C ₉ H ₁₁ NO ₃	60-18-4	181.188	2	25	9.11
<i>L</i> -Tyrosine	4-Hydroxy- <i>L</i> -phenylalanine	C ₉ H ₁₁ NO ₃	60-18-4	181.188	3	25	10.1
Tyrosineamide		C ₉ H ₁₂ N ₂ O ₂	4985-46-0	180.203		25	7.33
Undecylamine	1-Undecanamine	C ₁₁ H ₂₃ N	7307-55-3	171.324		25	10.63
Uracil		C ₄ H ₄ N ₂ O ₂	66-22-8	112.087		25	9.45
Urea	Carbamide	CH ₄ N ₂ O	57-13-6	60.055		25	0.10
Uric acid		C ₅ H ₄ N ₄ O ₃	69-93-2	168.111		12	3.89
5'-Uridylic acid	Uridine 5'-phosphoric acid	C ₉ H ₁₃ N ₂ O ₆ P	58-97-9	324.180	1		6.4
5'-Uridylic acid	Uridine 5'-phosphoric acid	C ₉ H ₁₃ N ₂ O ₆ P	58-97-9	324.180	2		9.5
<i>L</i> -Valine	2-Aminoisovaleric acid	C ₅ H ₁₁ NO ₂	72-18-4	117.147	1	25	2.29
<i>L</i> -Valine	2-Aminoisovaleric acid	C ₅ H ₁₁ NO ₂	72-18-4	117.147	2	25	9.74
Valium	7-Chloro-1,3-dihydro-1-methyl-5-phenyl-2 <i>H</i> -1,4-benzodiazepin-2-one	C ₁₆ H ₁₃ ClN ₂ O	439-14-5	284.739			3.4
Verapamil		C ₂₇ H ₃₈ N ₂ O ₄	52-53-9	454.602			8.6
Veratridine		C ₃₆ H ₅₁ NO ₁₁	71-62-5	673.790			9.54
Vinblastine		C ₄₆ H ₅₈ N ₄ O ₉	865-21-4	810.975	1		5.4
Vinblastine		C ₄₆ H ₅₈ N ₄ O ₉	865-21-4	810.975	2		7.4
Vincristine		C ₄₆ H ₅₆ N ₄ O ₁₀	57-22-7	824.958			5.4
Xanthopterin		C ₆ H ₅ N ₅ O ₂	119-44-8	179.137	2	20	6.59
Xanthopterin		C ₆ H ₅ N ₅ O ₂	119-44-8	179.137	3	20	9.31
<i>D</i> -Xylose		C ₅ H ₁₀ O ₅	58-86-6	150.130		18	12.14